Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Vibronic Optical Spectroscopy of Cryogenic Flavin Ions: The O2+ and N1 Tautomers of Protonated Lumiflavin

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Figure Captions

Figure S1. Photodissociation mass spectrum of H^+LF recorded for excitation wavelength of 23128 cm^{-1} (432.37 nm) assigned to the S_1 origin of the O2+ tautomer at a trap temperature of *T*=6 K. The branching ratio depends somewhat on the timing of the high-voltage extraction pulse of the reflectron time-of-flight mass spectrometer. In general, the branching ratio does not depend significantly on the excitation frequency, leading to essentially the same VISPD action spectra monitored in each fragment channel (Figure S2). The suggested assignment of the fragment peaks is provided in Table S1.

Figure S2. VISPD spectra of H^+LF recorded in various fragmentation channels measured at a trap temperature of T=6 K. The spikes between 20500 and 21000 cm^{-1} are not reproducible. The overview spectrum is recorded with the OPO laser at a step size of 0.5 nm (20 cm^{-1} at 500 nm).

Figure S3. Structures of the less stable protomers of H^+LF in the S_0 state obtained at the PBE0/cc-pVDZ level.

Figure S4. Vertical (S_1-S_4, T_1-T_4) excitation energies of various H^+LF protomers and LF with respect to the S_0 energy computed at the PBE0/cc-pVDZ level. Triplet energies are reported in Table S7.

Figure S5. Vertical (S_1-S_4) and adiabatic (S_1-S_2) excitation energies of various H^+LF protomers and LF with respect to S_0 computed at the PBE0/cc-pVDZ level.

Figure S6. Atomic NBO charge distribution in the S_0 and S_1 states of neutral LF (in 10^{-3} e) evaluated at the PBE0/cc-pVDZ level.

Figure S7. Schematic visualization of in-plane normal modes m1-m12 of LF in the S_1 state calculated at the PBE0/cc-pVDZ level.

Figure S8. Schematic visualization of in-plane normal modes m1-m12 of H^+LF(O2+) in the S_1 state calculated at the PBE0/cc-pVDZ level.

Figure S9. Laser-induced fluorescence excitation spectrum of the $S_1 \leftarrow S_0$ transition of LF in He droplets (Vdovin et al., Chem. Phys. **422**, 195 (2013)) compared to corresponding VISPD spectrum of H^+LF. Corresponding transitions are connected by dotted lines.

Figure S10. Schematic visualization of low energy out-of-plane modes (n1-n8) of H^+LF(N1) in the S_1 state calculated at the PBE0/cc-pVDZ level.

Figure S11. Comparison between Franck-Condon simulations for the $S_1 \leftarrow S_0$ transition of H^+LF(N1) with planar structure (transition state) and slightly bent structure (minimum).

Figure S12. Comparison between Franck-Condon simulations for the $S_1 \leftarrow S_0$ transition of various H^+LF protomers shown in Figure 1 and S3.

Figure S13: Absolute distances of neutral lumiflavin in its electronic ground state S_0. Geometry changes upon protonation (O2+/N1). Positive values indicate elongations, negative values indicate contractions. All values are given in pm.

Figure S14. Dependence of the intensity of the 0^0 transition of the H^+LF(O2+) protomer (top) and H^+LF(N1) protomer (bottom) as a function of the laser power. According to a least-square error analysis, the experimental data is better fitted by linear than a quadratic curve.

Figure S15. Comparison of VISPD spectrum of cryogenic H^+LF ins in the gas phase with absorption spectrum of LF and H^+LF in solution.

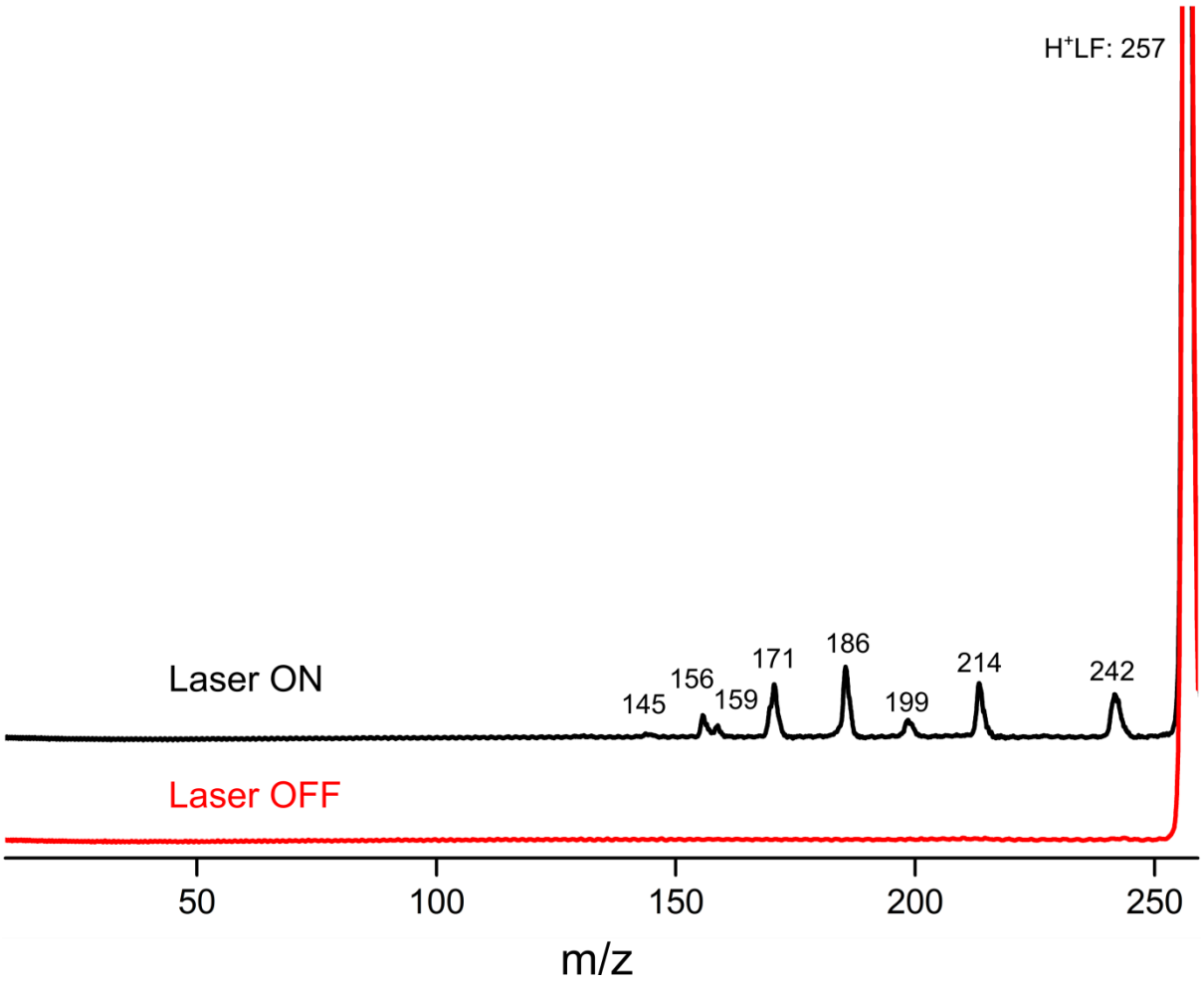

H+LF: 257
Laser ON
145
156
159
171
186
199
214
242
Laser OFF
50
100
150
200
250
m/z

Figure S1

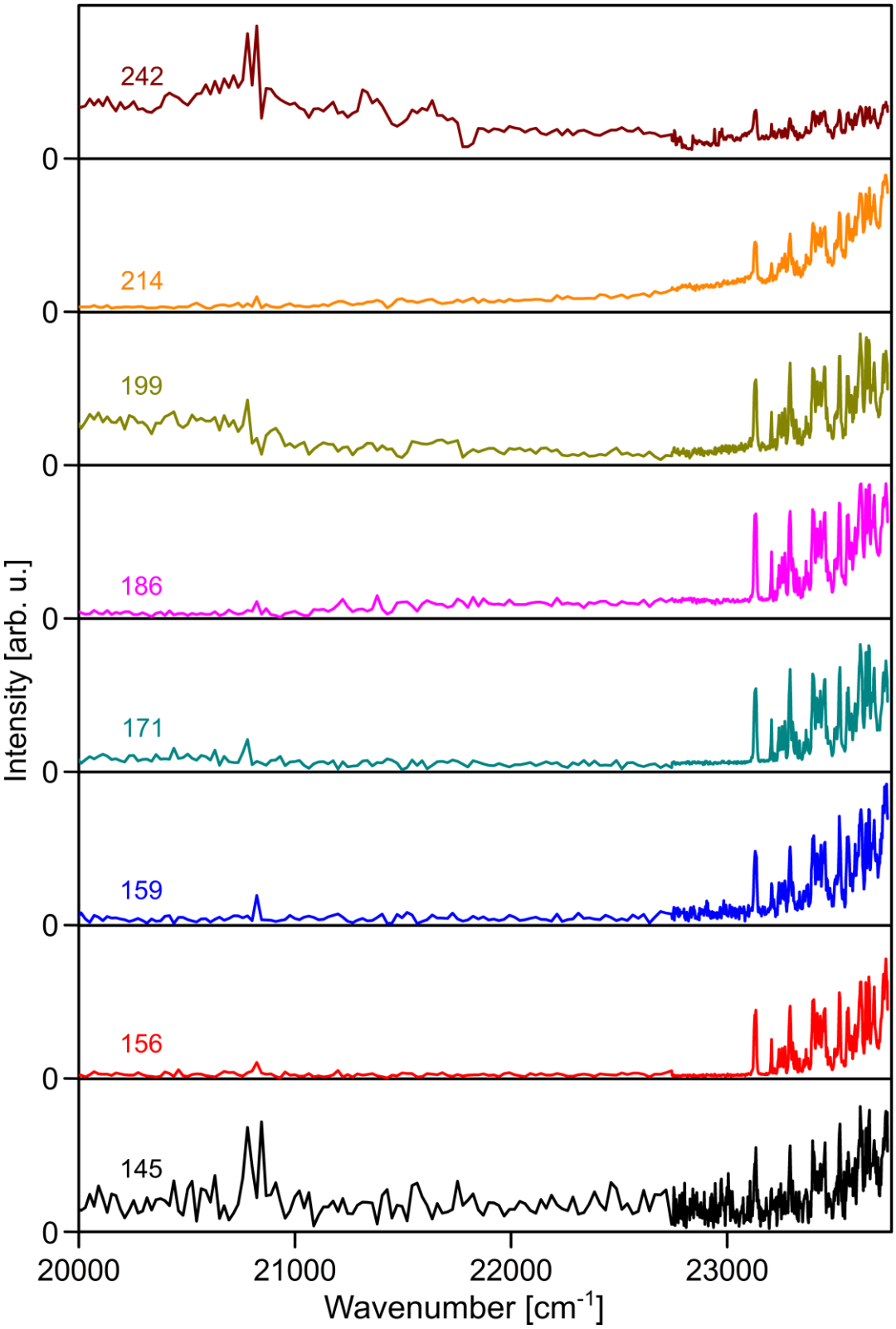

242
214
199
186
171
159
156
145
0
Intensity [arb. u.]
20000
21000
22000
23000
Wavenumber [cm-1]

Figure S2

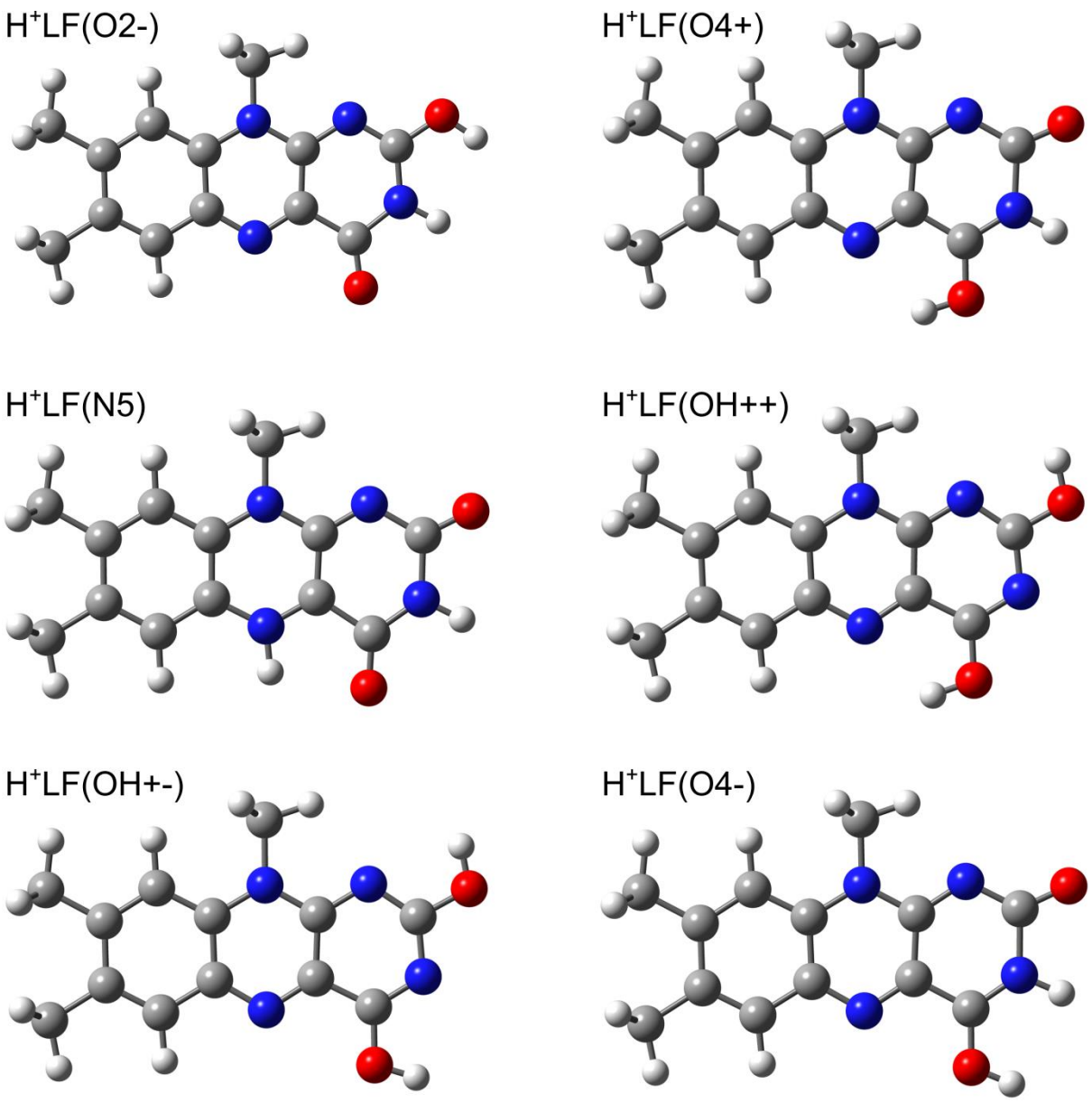


Figure S3

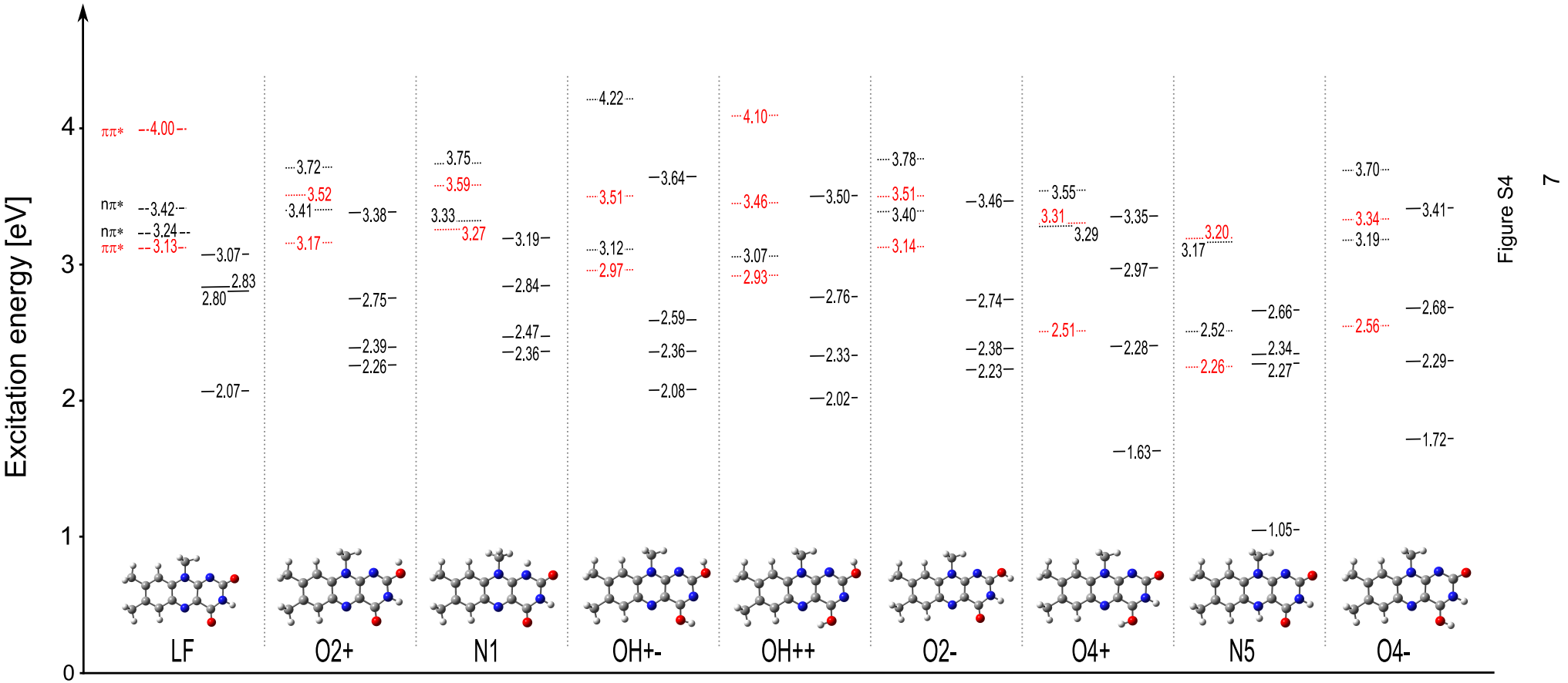

Excitation energy [eV]
0
1
2
3
4
ππ*
nπ*
nπ*
ππ*
4.00
3.42
3.24
3.13
3.07
2.83
2.80
2.07
LF
3.72
3.52
3.41
3.17
3.38
2.75
2.39
2.26
O2+
3.75
3.59
3.33
3.27
3.19
2.84
2.47
2.36
N1
4.22
3.51
3.12
2.97
3.64
2.59
2.36
2.08
OH+-
4.10
3.46
3.07
2.93
3.50
2.76
2.33
2.02
OH++
3.78
3.51
3.40
3.14
3.46
2.74
2.38
2.23
O2-
3.55
3.31
3.29
2.51
3.35
2.97
2.28
1.63
O4+
3.20
3.17
2.52
2.26
2.66
2.34
2.27
1.05
N5
3.70
3.34
3.19
2.56
3.41
2.68
2.29
1.72
O4-

Figure S4

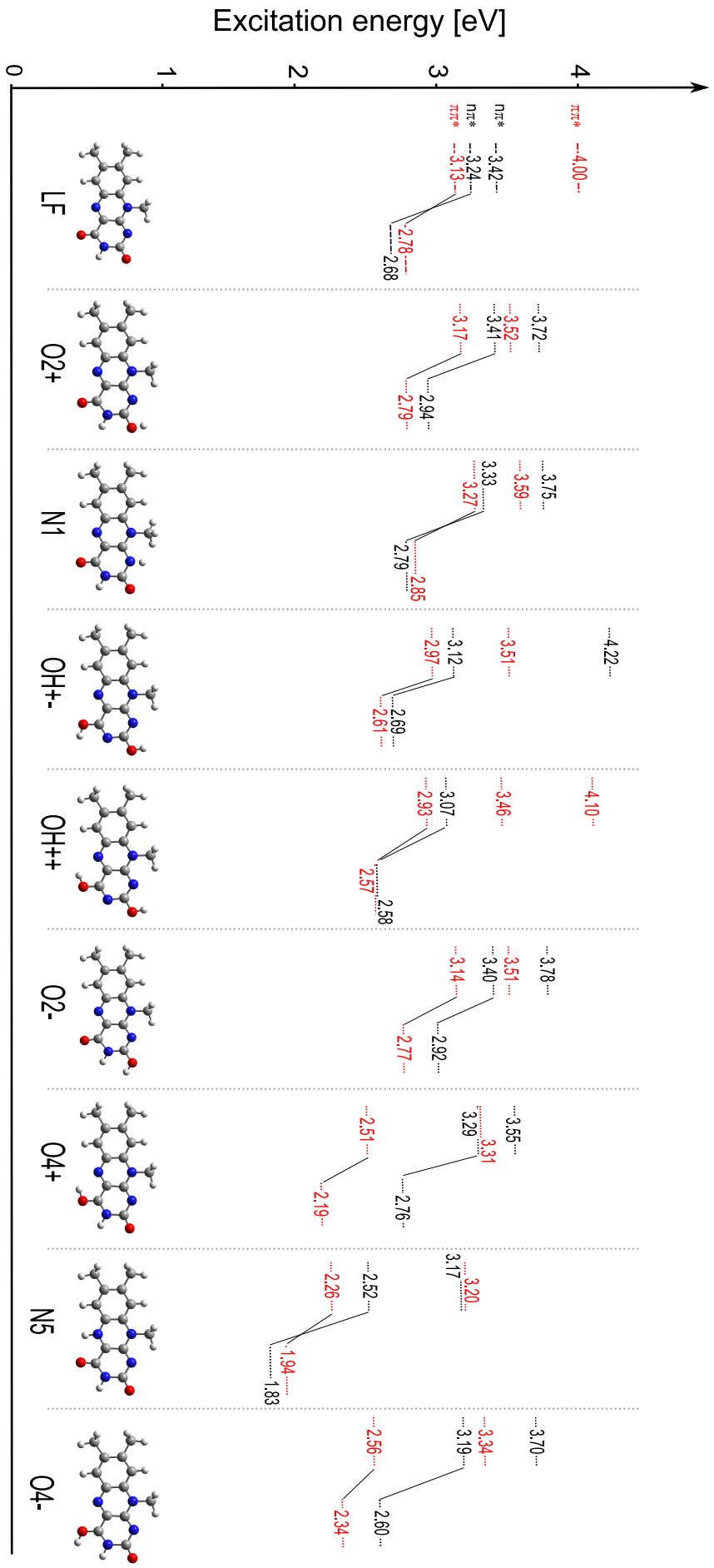

Excitation energy [eV]
0
1
2
3
4
LF
O2+
N1
OH+-
OH++
O2-
O4+
N5
O4-
ππ*
nπ*
nπ*
ππ*
4.00
3.42
3.24
3.13
2.78
2.68
3.72
3.52
3.41
3.17
2.94
2.79
3.75
3.59
3.33
3.27
2.79
2.85
4.22
3.51
3.12
2.97
2.69
2.61
4.10
3.46
3.07
2.93
2.57
2.58
3.78
3.51
3.40
3.14
2.92
2.77
3.55
3.31
3.29
2.76
2.51
2.19
3.70
3.20
3.17
2.52
2.26
1.94
1.83
3.70
3.34
3.19
2.60
2.56
2.34

Figure S5

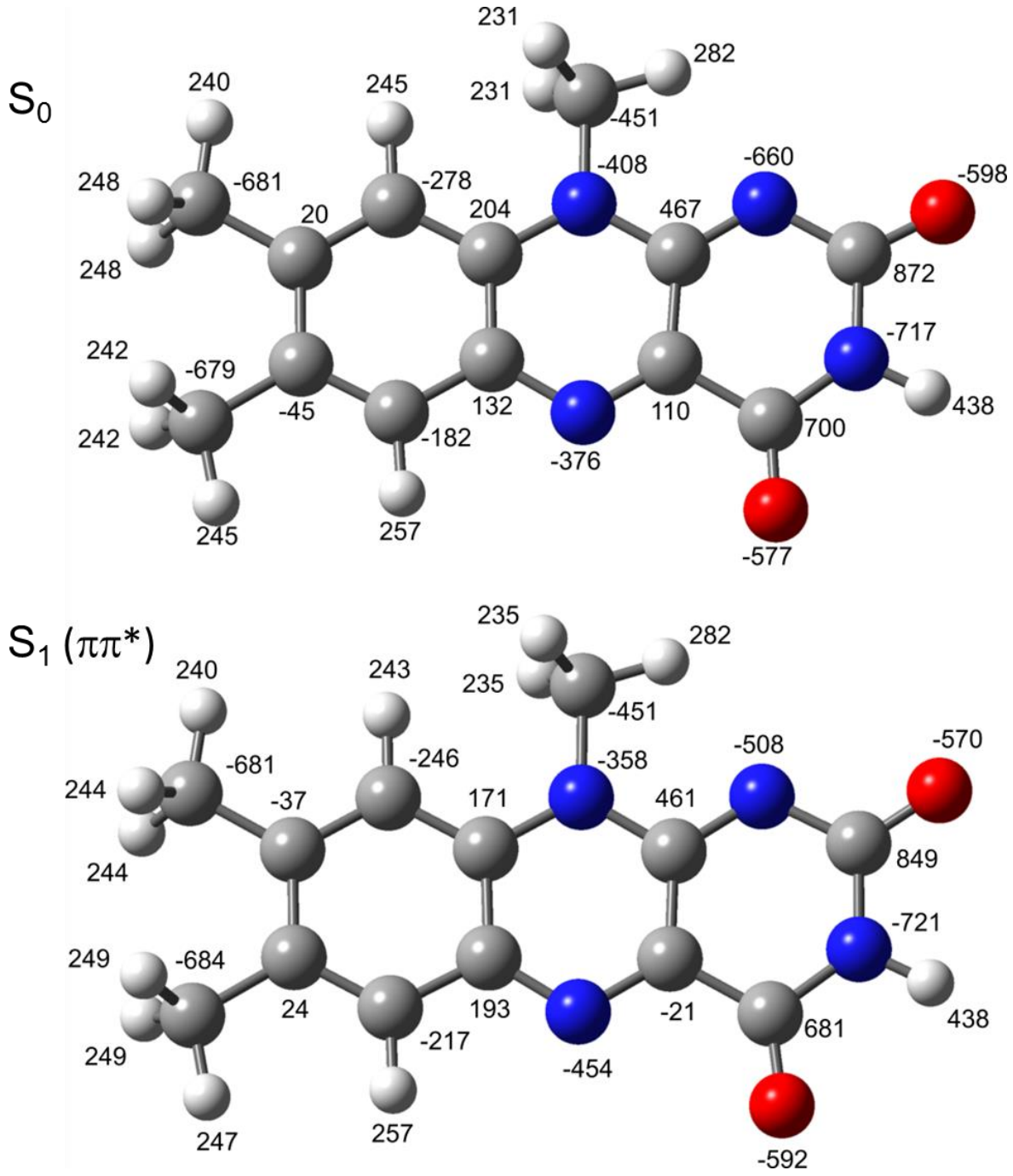

S0
231
282
240
245
231
-451
-408
-660
-598
248
-681
-278
20
204
467
872
248
-717
242
-679
438
-45
132
110
700
242
-182
-376
245
257
-577
S1 (ππ*)
235
282
240
243
235
-451
-508
-570
-681
-246
-358
244
-37
171
461
849
244
-721
249
-684
24
193
-21
438
681
249
-217
-454
247
257
-592

Figure S6

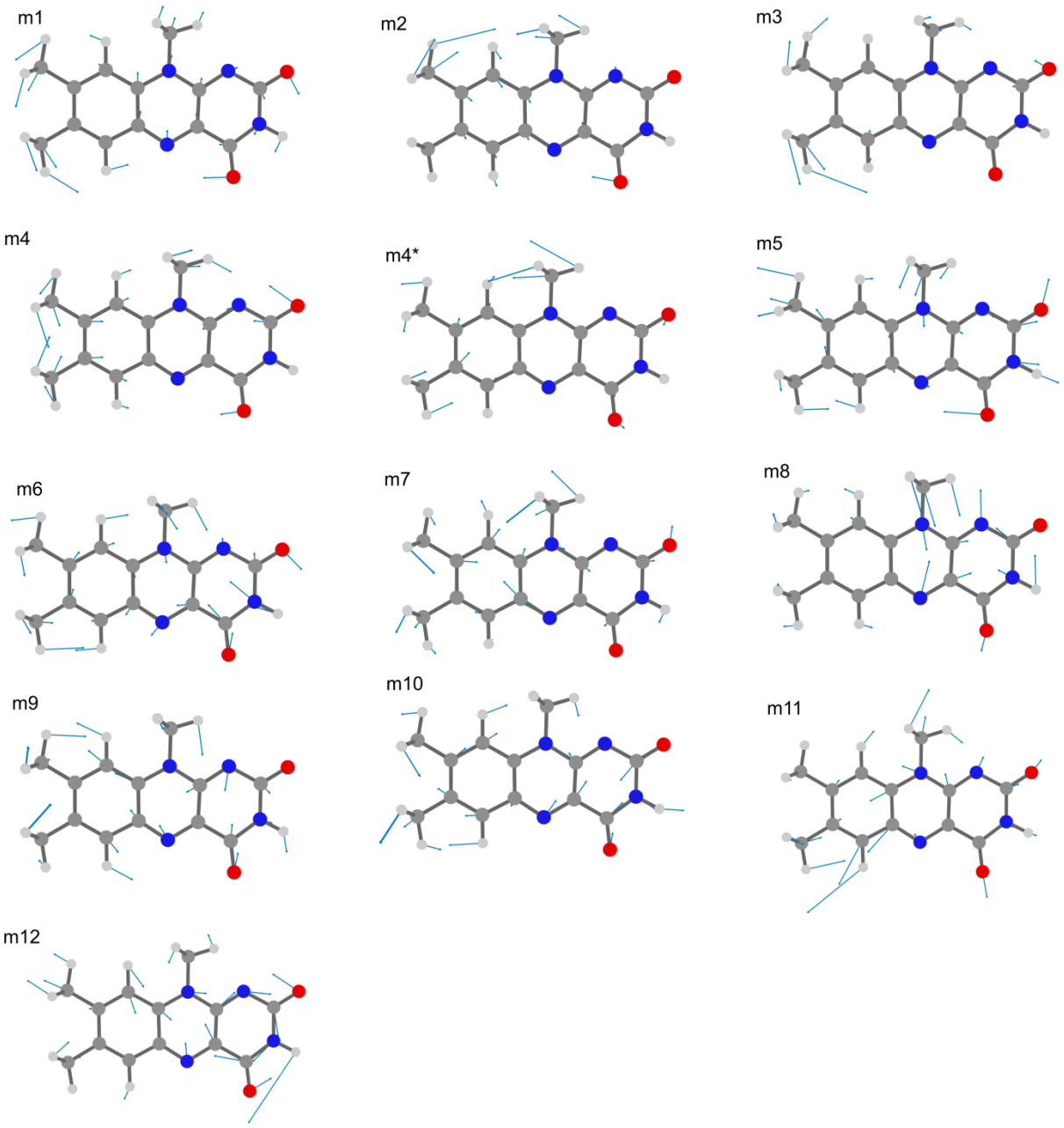


Figure S7

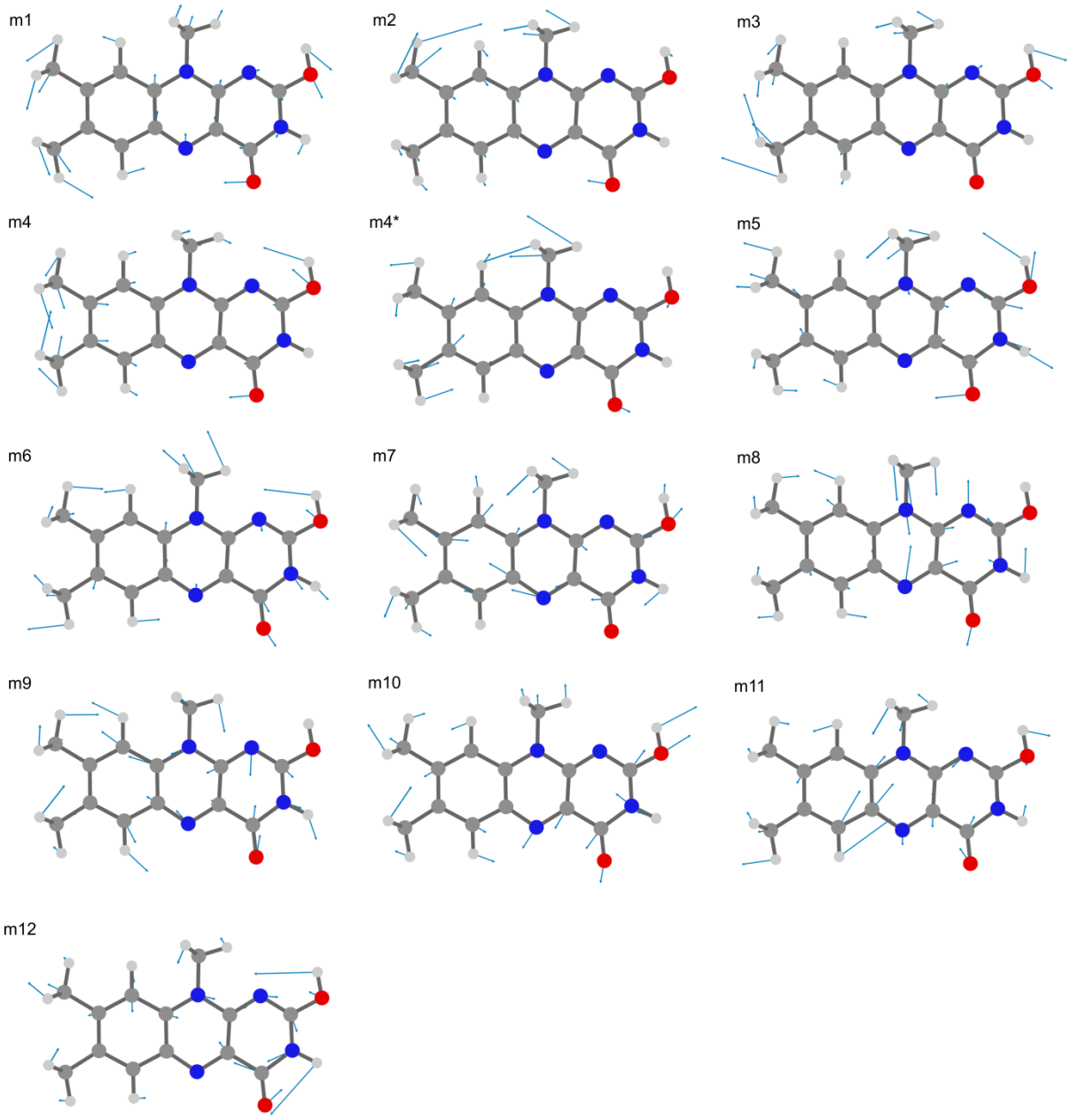


Figure S8

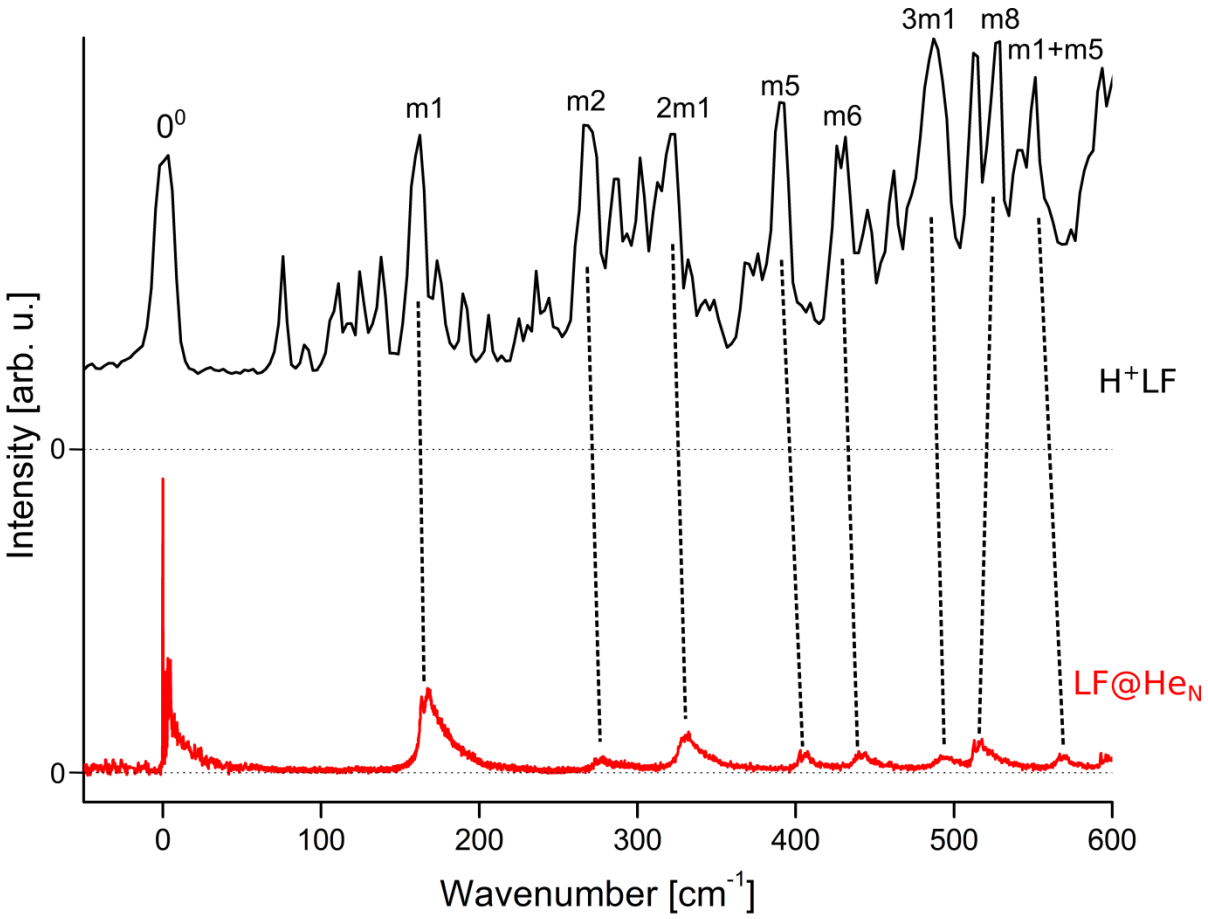

3m1
m8
m1+m5
m5
m6
2m1
m2
m1
0⁰
H⁺LF
LF@He_N
Intensity [arb. u.]
0
0
0
100
200
300
400
500
600
Wavenumber [cm⁻¹]

Figure S9

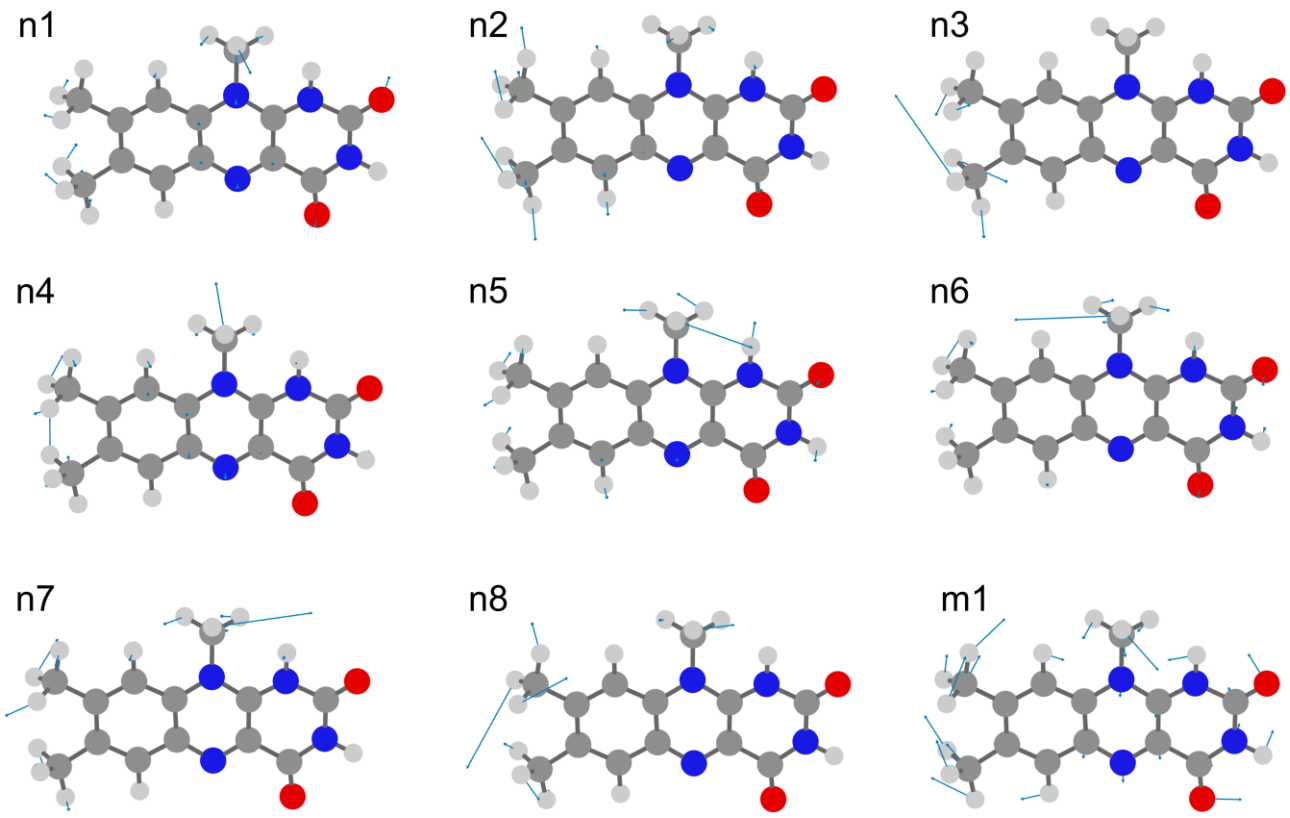


Figure S10

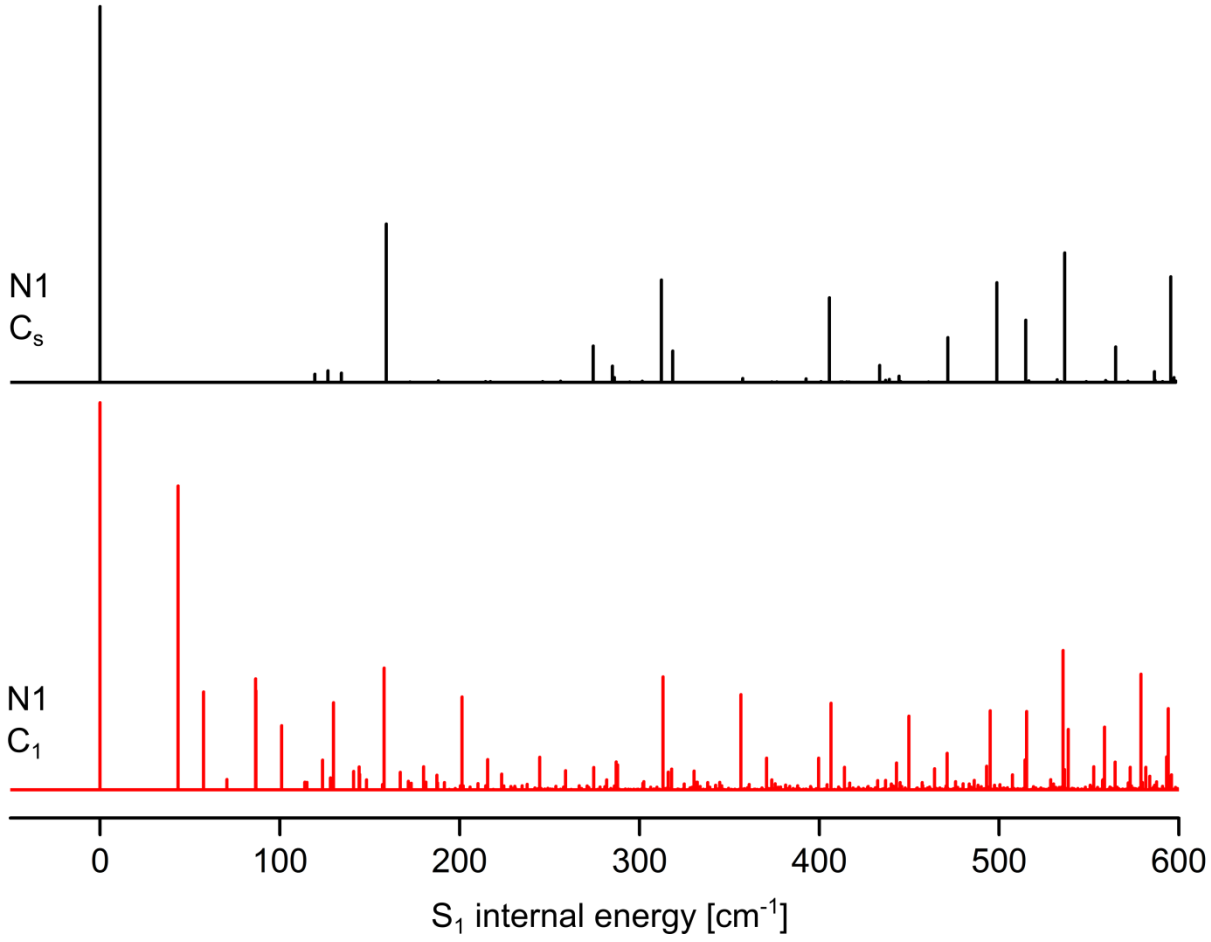


Figure S11

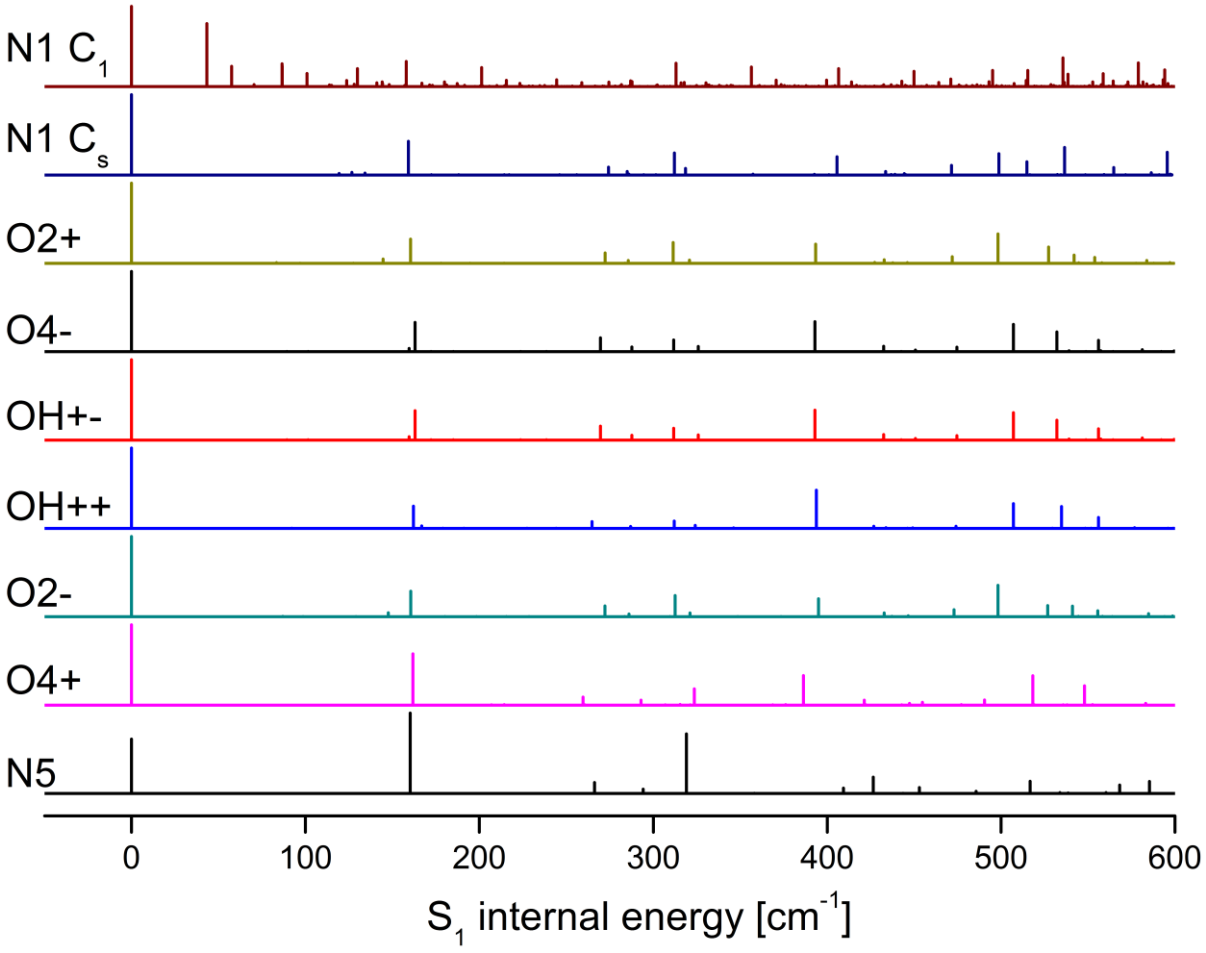

N1 C1
N1 Cs
O2+
O4-
OH+-
OH++
O2-
O4+
N5
0
100
200
300
400
500
600
S1 internal energy [cm-1]

Figure S12

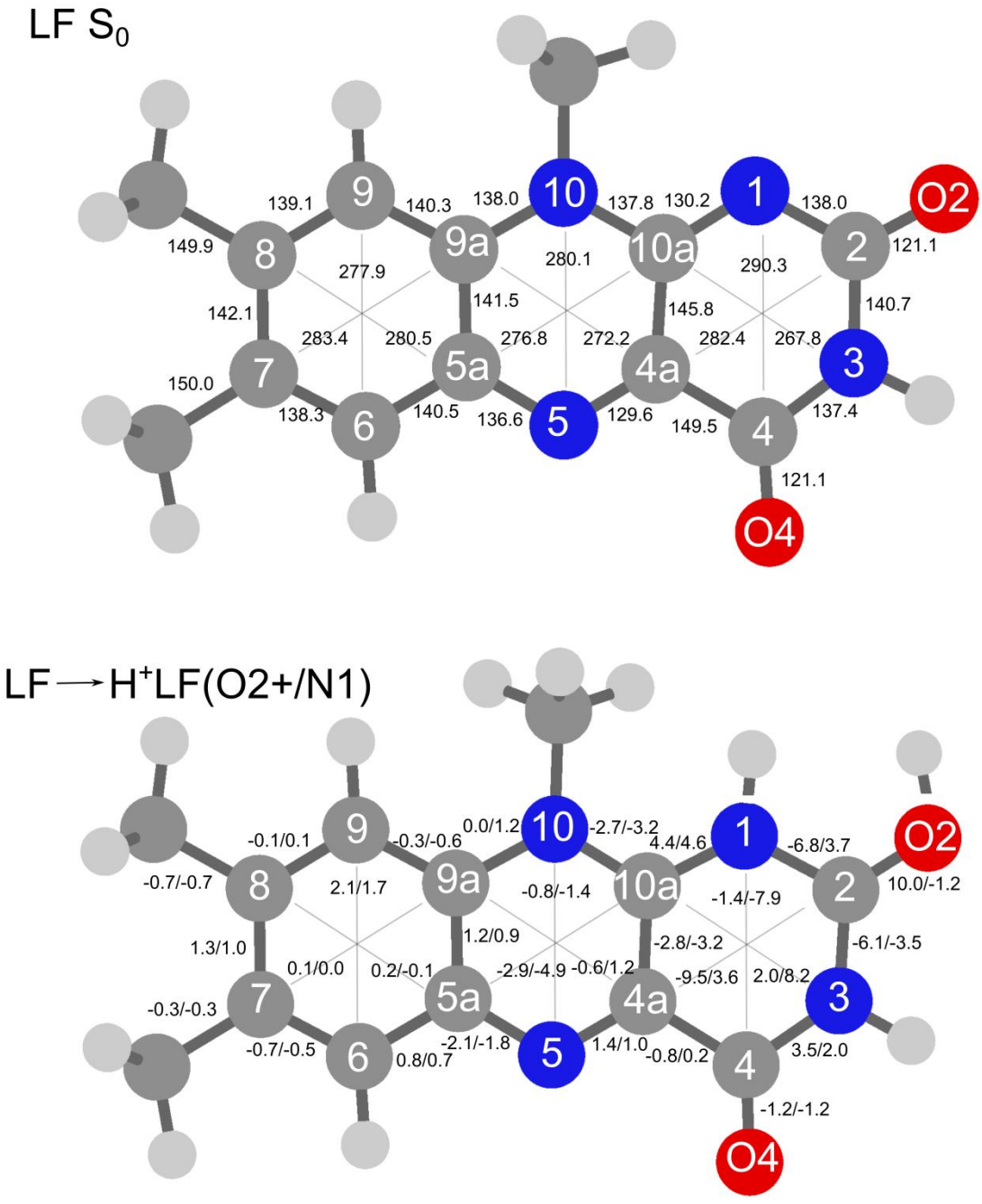
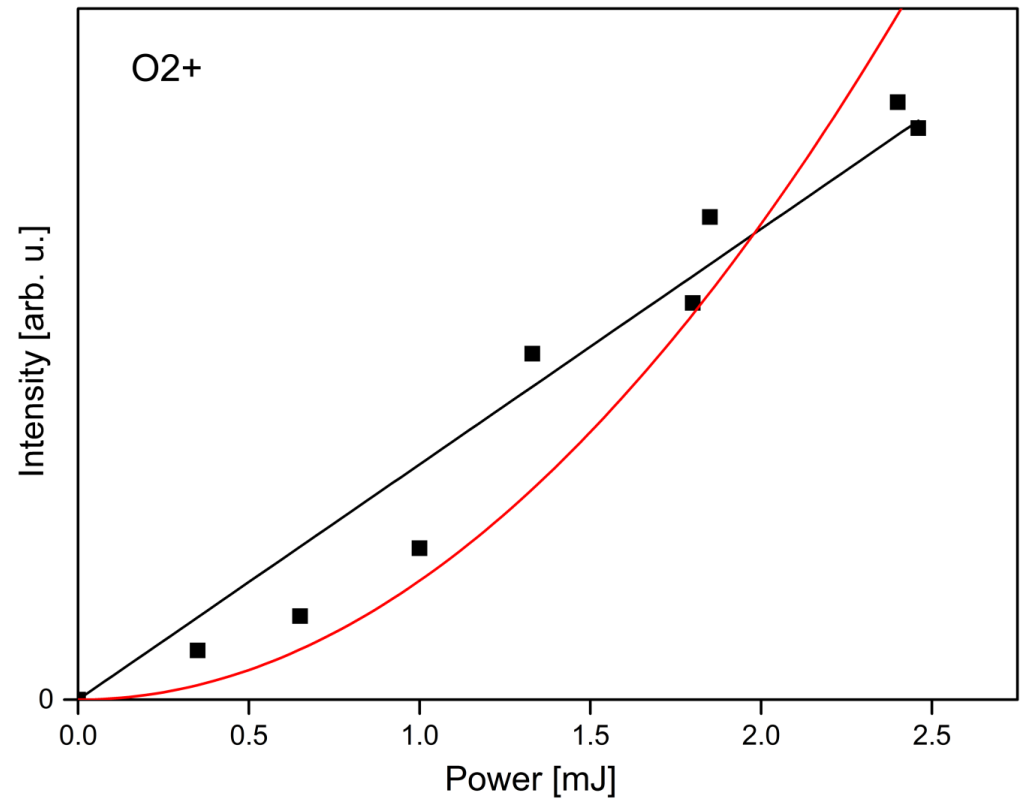

LF S_0
9
10
1
O2
8
9a
10a
2
7
5a
4a
3
6
5
4
O4
139.1
140.3
138.0
137.8
130.2
138.0
121.1
149.9
277.9
280.1
290.3
141.5
145.8
140.7
142.1
283.4
280.5
276.8
272.2
282.4
267.8
150.0
138.3
140.5
136.6
129.6
149.5
137.4
121.1
LF⟶H⁺LF(O2+/N1)
-0.1/0.1
0.0/1.2
-2.7/-3.2
4.4/4.6
-6.8/3.7
-0.3/-0.6
-0.7/-0.7
2.1/1.7
-0.8/-1.4
-1.4/-7.9
10.0/-1.2
1.3/1.0
1.2/0.9
-2.8/-3.2
-6.1/-3.5
0.1/0.0
0.2/-0.1
-2.9/-4.9
-0.6/1.2
-9.5/3.6
2.0/8.2
-0.3/-0.3
-0.7/-0.5
-2.1/-1.8
1.4/1.0
-0.8/0.2
3.5/2.0
0.8/0.7
-1.2/-1.2

Figure S13


O2+
Intensity [arb. u.]
0
0.0
0.5
1.0
1.5
2.0
2.5
Power [mJ]

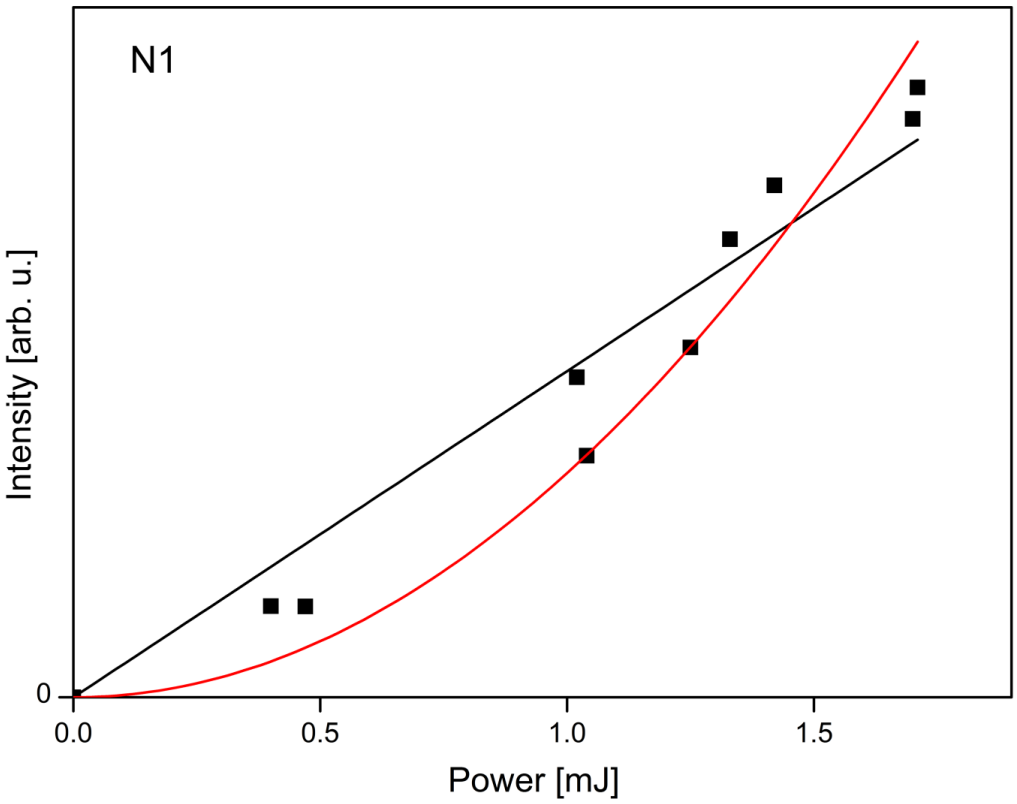

N1
Intensity [arb. u.]
0
0.0
0.5
1.0
1.5
Power [mJ]

Figure S14

Tyagi et al. J. Photochem. Photobiol. A Chem. **215** (2010)

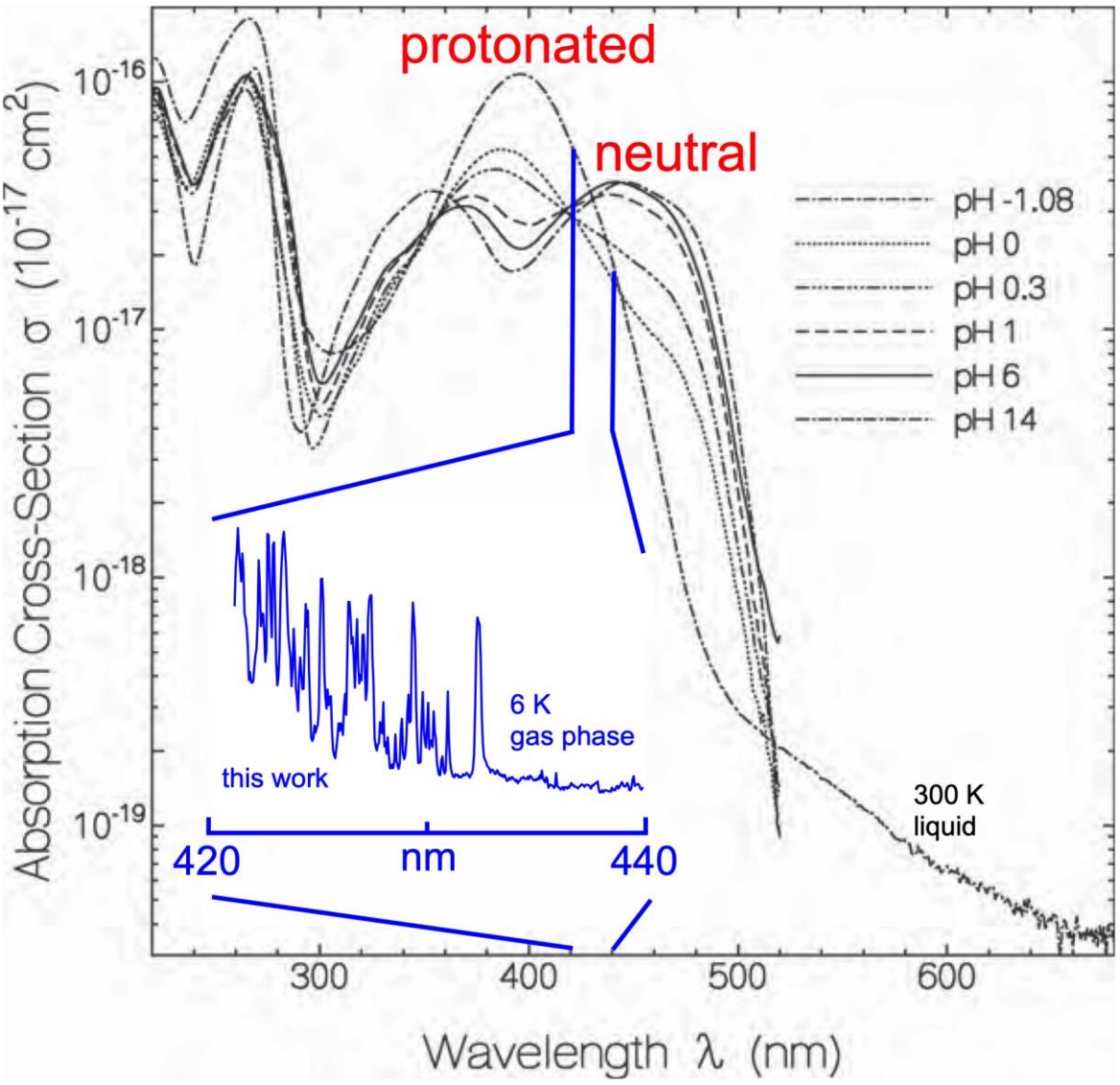


Figure S15

Table S1. Fragmentation channels of H^+LF (m/z 257) observed upon VISPD and possible assignment of neutral fragment molecules.

Fragment Ion (m/z)	Assignment	Loss from H^+LF (m/z)
145	$2CO + CH_3CN + CH_3$ $CO + CH_3CN + OCNH$	112
156	$OCNH + CO + 2CH_3$	101
159	OCNH + CO + HCN	98
171	$OCNH + CO + CH_3$	86
186	OCNH + CO	71
199	CH_3 + OCNH CO + 2 CH3	58
214	$CO + CH_3$ OCNH	43
242	CH3	15

Table S2. Selected atomic charges (in e) of H^+LF(O2+/N1) and LF for the S_0 and S_1 states using natural bond orbital analysis (PBE0/cc-pVDZ).

	q_H		q_{N5}		q_{O4}		q_{O2}		q_{N1}	
	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1	S_0	S_1
O2+	0.521	0.517	-0.336	-0.457	-0.507	-0.533	-0.639	-0.645	-0.671	-0.655
N1	0.462	0.457	-0.327	-0.456	-0.508	-0.530	-0.555	-0.574	-0.671	-0.659
LF			-0.376	-0.454	-0.577	-0.592	-0.598	-0.570	-0.660	-0.508

Table S3. Calculated frequencies (in cm^{-1}) of $H^+LF(O2+)$ for the S_0 and S_1 states at the PBE0/cc-pVDZ level of theory. Frequencies are listed according to symmetry following the Mullikan notation.

S_0		S_1	
a''	**a'**	**a''**	**a'**
50.91	164.25	41.67	160.42
61.00	281.26	55.14	272.39
102.56	298.26	72.36	285.68
134.29	322.24	88.95	311.49
149.23	357.74	141.89	348.26
164.24	398.21	152.99	393.39
177.48	431	158.43	427.30
193.66	497.66	176.05	498.28
207.08	531.75	195.42	527.39
266.53	548.9	218.89	541.95
347.46	603.25	311.51	603.27
400.17	642.12	346.47	631.04
465.55	650.26	388.87	647.84
536.68	758.05	453.14	747.29
562.93	790.12	537.15	787.16
639.88	838.75	586.08	830.83
675.21	894.65	640.79	893.72
731.54	998.83	697.71	992.97
757.96	1023.89	737.35	1007.58
782.37	1030.1	743.71	1026.94
837.02	1090.02	793.81	1080.10
868.33	1112.68	871.33	1103.48
921.80	1176.55	900.03	1166.80
1029.66	1184.46	990.18	1177.52
1053.37	1214.26	1039.02	1208.38
1133.92	1248.13	1127.24	1229.47
1438.16	1261.77	1413.95	1255.73
1454.48	1309.35	1449.42	1272.21
1472.41	1329.83	1474.99	1319.26
3134.36	1354.52	3089.84	1342.48
3138.27	1372.71	3134.53	1351.39
3186.33	1384.95	3152.86	1361.99
	1395.14		1382.53
	1405.22		1392.81
	1426.54		1400.65
	1432.96		1414.90
	1452.65		1442.95
	1464.6		1450.31
	1482.7		1464.76
	1506.29		1470.27
	1545.15		1485.36
	1550.12		1526.85
	1620.26		1564.94
	1634.99		1595.28
	1650.21		1635.10
	1681.71		1664.09
	1700.67		1703.13
	1889.33		1855.31
	3062.16		3031.46
	3064.36		3060.97
	3092.97		3068.84
	3180.5		3177.19
	3181.28		3188.41
	3235.34		3227.03
	3246.62		3230.26
	3249.32		3240.20
	3586.67		3590.35
	3770.09		3779.48

Table S4. Calculated frequencies (in cm^{-1}) of $H^+LF(N1)$ for the S_0 and S_1 state at the PBE0/cc-pVDZ level of theory.

S_0 a''	S_1 a''
47.25	43.30
61.67	57.56
97.64	70.49
105.55	86.50
132.34	123.69
133.59	132.29
140.89	144.39
163.27	148.19
181.45	157.98
199.12	179.96
249.75	197.55
289.00	274.56
298.62	287.08
324.23	287.96
339.66	313.11
374.94	333.72
388.29	365.56
410.95	378.50
431.05	406.63
457.31	427.19
498.21	440.13
517.34	495.11
525.77	515.37
543.62	535.64
572.52	547.93
596.63	583.82
630.98	594.13
637.87	614.55
660.74	629.07
666.82	659.90
720.19	686.67
756.04	714.76
764.55	745.19
774.40	761.75
786.51	780.88
820.71	786.29
841.61	836.09
862.58	871.07
879.21	877.60
923.12	895.66
996.67	985.61
1017.54	990.16
1025.43	1005.42
1028.87	1013.45
1035.83	1035.68
1053.19	1039.94
1109.51	1101.67
1121.85	1117.14
1183.01	1175.21
1196.61	1181.11
1228.29	1213.63
1266.79	1259.28
1295.22	1271.74
1306.95	1304.47
1349.22	1331.30
1366.03	1333.91
1383.21	1343.32
1392.52	1378.12
1400.55	1379.92
1424.64	1396.92
1430.40	1408.50
1435.61	1416.17
1437.69	1421.82
1438.94	1440.41
1454.55	1449.43
1458.87	1461.92
1469.58	1467.76
1493.96	1470.65
1496.71	1479.05
1519.79	1486.87
1563.24	1524.46
1573.27	1566.79
1630.79	1590.04
1675.56	1636.99
1701.75	1686.57
1882.05	1856.35
1909.16	1893.05
3062.37	3026.97
3065.09	3062.42
3088.26	3062.60
3134.91	3083.74
3139.56	3136.88
3180.47	3161.58
3182.29	3177.82
3188.52	3190.58
3223.75	3192.89
3235.85	3226.62
3246.27	3233.83
3596.50	3606.75
3630.52	3634.84

Table S5. Possible peak assignment of the sharp peaks a-t in the VISPD spectrum of H^+LF to low-frequency a" modes of the H^+LF(O2+) isomer.

Peak	Exp	Calc O2+	a" modes
	75	83, 72	2x42, 72
a	90	97, 89	42+55, 89
b	104	97	42+55
c	110/111	110	2x55
d	117	114	42+72
e	124	131	42+89
f	127	131	42+89
g	132	131	42+89
h	138	144	55+89
i	165	161	72+89
j	174/176	178	2x89
k	180	178	2x89
l	190	195	153+42
m	206	200	158+42
n	214	214	158+55, 142+72
o	225	225	153+72
p	231	231	158+72, 89+142, 55+176
q	237	237	195+42
r	241	242	153+89
s	245	247	158+89
t	262	261	219+42

Table S6. Adiabatic S_1 energies of LC, LF, and various protonated tautomers computed at the PBE0/cc-pVDZ level compared to available experimental values (in cm^{-1}).

tautomer	H^+LC (S_1) calc[a]	H^+LC (S_1) exp[a]	H^+LF (S_1) calc	H^+LF (S_1) exp
neutral	24826		22448	21511[b]
N1	-	-	23025	23202
O2+	22422		22535	23128
O2-			22341	
O4+	18451		17682	
O4-			18046	
N5	19153	19962	15622	
N10	22555		-	-

[a] Sheldrick et al., Phys. Chem. Chem. Phys. **20**, 7407 (2018)
[b] Vdovin et al., Chem. Phys. **422**, 195 (2013)

Table S7. Vertical and adiabatic triplet excitation energies computed at the PBE0/cc-pVDZ level with respect to the optimized electronic ground state S_0 (in cm^{-1}).

	T_1	T_2	T_3	T_4
	E_v (E_a)	E_v	E_v	E_v
LF	16699	22605	22791	24748
O2+	18250 (16522)	19301	22186	27250
N1	19009 (17413)	19957	22906	25715
O2-	17947 (16258)	19215	22135	27898
O4+	13175 (11803)	18361	23981	26980
N5	8469 (7745)	18280	18910	21491
OH++	16266 (14615)	18765	22281	28217
OH+-	16743 (15005)	19073	20896	29350
O4-	16743 (12372)	19073	20896	29350

Table S8. Optimized geometries of S_0-S_2 of LF and H^+LF shown in Figure 1 and Figure S3

LF S_0

C	3.38348600	0.85042200	-0.00001600
C	2.16039400	1.49512100	-0.00003800
C	0.94383400	0.78947700	-0.00002300
C	0.96364100	-0.62542700	0.00001400
C	2.20235500	-1.28386500	0.00003900
C	3.39646100	-0.57089900	0.00002400
C	-1.43638600	-0.62289000	0.00001000
C	-1.33517300	0.83160900	-0.00002800
C	-2.61876800	1.59714400	-0.00005000
C	-3.75101300	-0.63136900	0.00001400
H	2.09192200	2.58466300	-0.00006900
H	-4.62871600	1.22926700	-0.00003400
N	-0.23791700	-1.30367400	0.00002700
N	-2.54596300	-1.30467200	0.00003100
N	-3.71992900	0.77525500	-0.00002400
N	-0.22368300	1.49765300	-0.00004500
O	-2.68970000	2.80593600	-0.00007600
O	-4.82340100	-1.19474600	0.00003000
C	4.70096100	-1.30875100	0.00004800
H	5.30637400	-1.04711900	0.88291200
H	4.55111300	-2.39638200	0.00013700
H	5.30632200	-1.04725900	-0.88289400
C	4.66497100	1.62989100	-0.00002700
H	5.28059200	1.39850400	0.88434000
H	5.28067800	1.39834400	-0.88429000
H	4.46900600	2.71018700	-0.00013200
H	0.24896700	-3.14193000	0.89746000
C	-0.25734700	-2.75829400	0.00006200
H	-1.30700300	-3.06833300	0.00005100
H	0.24900100	-3.14197200	-0.89729800
H	2.24450900	-2.37242900	0.00007100

Sum of electronic and zero-point Energies= -870.962549
Sum of electronic and thermal Energies= -870.946653
Sum of electronic and thermal Enthalpies= -870.945708
Sum of electronic and thermal Free Energies= -871.005463

LF S_1

C	3.38995800	0.83517600	-0.00001600
C	2.17233200	1.50837000	-0.00003500
C	0.92872600	0.84540600	-0.00001800
C	0.96735000	-0.59631300	0.00002300
C	2.19824700	-1.27370000	0.00004300
C	3.40955600	-0.59124400	0.00002400
C	-1.41105700	-0.55920500	0.00001800
C	-1.35859600	0.86358800	-0.00001800
C	-2.62630000	1.57782700	-0.00002500
C	-3.75333900	-0.64568400	-0.00000300
H	2.13668200	2.59913700	-0.00006600
H	-4.65063100	1.18868000	-0.00006100
N	-0.23642300	-1.27166700	0.00004000
N	-2.51875800	-1.29827300	0.00002900
N	-3.74553000	0.72957900	-0.00003100
N	-0.20134400	1.56862600	-0.00003700
O	-2.77116600	2.78544800	-0.00009700
O	-4.78578300	-1.29253500	0.00000300
C	4.70573500	-1.34114300	0.00004600
H	5.31884800	-1.09640700	0.88355600
H	4.53863900	-2.42681500	0.00008600
H	5.31884000	-1.09647200	-0.88348700
C	4.67190500	1.60455700	-0.00003500
H	5.28542100	1.35750000	0.88238700
H	5.28543600	1.35743300	-0.88242900
H	4.49070500	2.68685500	-0.00007700
H	0.25653000	-3.10295000	0.89629100
C	-0.25808700	-2.72668700	0.00007900
H	-1.30302300	-3.04734700	0.00008500
H	0.25653500	-3.10299800	-0.89610900
H	2.21741800	-2.36347200	0.00007400

Sum of electronic and zero-point Energies= -870.860269
Sum of electronic and thermal Energies= -870.844696
Sum of electronic and thermal Enthalpies= -870.843752
Sum of electronic and thermal Free Energies= -870.902746

LF S_2

C	3.39693900	0.84006400	-0.00001200
C	2.18502300	1.50613400	-0.00003100
C	0.93926900	0.82991700	-0.00001500
C	0.96839600	-0.59818100	0.00002500
C	2.19064400	-1.26981900	0.00004200
C	3.40469800	-0.57832100	0.00002500
C	-1.42208400	-0.57612200	0.00002200
C	-1.34713700	0.83040500	-0.00002600
C	-2.59652900	1.56146600	-0.00005900
C	-3.68138900	-0.63452500	-0.00002000
H	2.14010700	2.59665400	-0.00006100
H	-4.64503300	1.19663900	-0.00005800
N	-0.25124800	-1.27864100	0.00004600
N	-2.56083400	-1.31203800	0.00002400
N	-3.74541700	0.72642000	-0.00005800
N	-0.19485300	1.54532800	-0.00003900
O	-2.77545800	2.76173300	-0.00007600
O	-4.83444700	-1.19476900	0.00001700
C	4.69802900	-1.33530400	0.00004500
H	5.31187100	-1.09064100	0.88301400
H	4.52828800	-2.42066200	0.00007100
H	5.31187300	-1.09068400	-0.88293400
C	4.68675800	1.60694400	-0.00003200
H	5.29980900	1.36669900	0.88394800
H	5.29980200	1.36666400	-0.88400700
H	4.50353300	2.68953800	-0.00005300
H	0.25468800	-3.10864300	0.89528000
C	-0.26087200	-2.72926600	0.00009400
H	-1.30190200	-3.06113900	0.00011800
H	0.25466200	-3.10870400	-0.89508200
H	2.21754100	-2.35925600	0.00007000

Sum of electronic and zero-point Energies= -870.864040
Sum of electronic and thermal Energies= -870.847986
Sum of electronic and thermal Enthalpies= -870.847042
Sum of electronic and thermal Free Energies= -870.906828

H^+LF(O2+) S_0

C	-2.53002800	2.45026300	0.00000000
C	-2.44872100	1.07629800	0.00000000
C	-1.20394500	0.40467500	0.00000000
C	0.00000000	1.17105600	0.00000000
C	-0.07997400	2.56900100	0.00000000
C	-1.31324400	3.20929900	0.00000000
C	1.22491700	-0.86058100	0.00000000
C	-0.03132600	-1.54458600	0.00000000
C	-0.02418700	-3.03109800	0.00000000
C	2.39290000	-2.79758400	0.00000000
H	-3.34203400	0.44970600	0.00000000
H	0.82194000	3.17881900	0.00000000
H	1.37163900	-4.57308500	0.00000000
N	1.20259300	0.49378500	0.00000000
N	2.41685800	-1.48606700	0.00000000
N	1.28213300	-3.55821800	0.00000000
N	-1.19389000	-0.93979100	0.00000000
O	-0.98775500	-3.74381300	0.00000000
O	3.51106200	-3.48167200	0.00000000
C	-1.37105900	4.70150900	0.00000000
H	-1.91839300	5.07150000	0.88170100
H	-0.37091900	5.15190500	0.00000000
H	-1.91839300	5.07150000	-0.88170100
C	-3.85624500	3.14294900	0.00000000
H	-3.96819500	3.79003400	0.88414800
H	-3.96819500	3.79003400	-0.88414800
H	-4.68153200	2.42037600	0.00000000
H	2.50065800	1.87866500	0.89839300
C	2.45645700	1.24917900	0.00000000
H	3.28555700	0.53914300	0.00000000
H	2.50065800	1.87866500	-0.89839300
H	4.25361900	-2.85361400	0.00000000

Sum of electronic and zero-point Energies= -871.332633
Sum of electronic and thermal Energies= -871.316667
Sum of electronic and thermal Enthalpies= -871.315723
Sum of electronic and thermal Free Energies= -871.375306

H^+LF(O2+) S_1

C	-2.44955800	2.57754500	0.00000000
C	-2.38814500	1.14606900	0.00000000
C	-1.18671000	0.40804300	0.00000000
C	0.00000000	1.13847000	0.00000000
C	-0.05160500	2.57736200	0.00000000
C	-1.24242800	3.30314000	0.00000000
C	1.17215600	-0.92537900	0.00000000
C	-0.08457300	-1.57454400	0.00000000
C	-0.09085900	-3.04570000	0.00000000
C	2.33199400	-2.86883400	0.00000000
H	-3.31439500	0.56584700	0.00000000
H	0.88606800	3.13413200	0.00000000
H	1.27558000	-4.61758100	0.00000000
N	1.20562800	0.46794600	0.00000000
N	2.35732100	-1.55119300	0.00000000
N	1.21399400	-3.60097400	0.00000000
N	-1.27062500	-0.95475500	0.00000000
O	-1.05853600	-3.76247400	0.00000000
O	3.45358000	-3.55505600	0.00000000
C	-1.23167500	4.79923800	0.00000000
H	-1.74980100	5.20198100	0.88489000
H	-0.20828200	5.19501800	0.00000000
H	-1.74980100	5.20198100	-0.88489000
C	-3.76836400	3.25193900	0.00000000
H	-3.86612900	3.91709000	0.87698600
H	-3.86612900	3.91709000	-0.87698600
H	-4.60388800	2.54257600	0.00000000
H	2.56174700	1.80880700	0.89990100
C	2.47313700	1.18250000	0.00000000
H	3.27634700	0.44175300	0.00000000
H	2.56174700	1.80880700	-0.89990100
H	4.19214100	-2.92352300	0.00000000

Sum of electronic and zero-point Energies= -871.229954
Sum of electronic and thermal Energies= -871.213184
Sum of electronic and thermal Enthalpies= -871.212239
Sum of electronic and thermal Free Energies= -871.274094

H^+LF(O2+) S_2

C	-2.48994700	2.55460200	0.00000000
C	-2.46703400	1.16748100	0.00000000
C	-1.25104000	0.46792000	0.00000000
C	0.00000000	1.18076700	0.00000000
C	-0.05388100	2.56873800	0.00000000
C	-1.26514200	3.26999800	0.00000000
C	1.20141000	-0.91963800	0.00000000
C	-0.03746700	-1.60910100	0.00000000
C	-0.06840700	-3.07417100	0.00000000
C	2.35253700	-2.88139000	0.00000000
H	-3.38939100	0.58669700	0.00000000
H	0.87386500	3.14028900	0.00000000
H	1.29150400	-4.63274800	0.00000000
N	1.19328500	0.44992200	0.00000000
N	2.37433700	-1.57304500	0.00000000
N	1.22687800	-3.61637100	0.00000000
N	-1.11467800	-0.84914800	0.00000000
O	-1.05706400	-3.76372700	0.00000000
O	3.46383300	-3.58203300	0.00000000
C	-1.25855200	4.76502500	0.00000000
H	-1.78307900	5.16476300	0.88279400
H	-0.23791400	5.16792100	0.00000000
H	-1.78307900	5.16476300	-0.88279400
C	-3.79798300	3.28201300	0.00000000
H	-3.88815100	3.93286700	0.88392700
H	-3.88815100	3.93286700	-0.88392700
H	-4.64658700	2.58689400	0.00000000
H	2.51749900	1.81281700	0.89821500
C	2.45423200	1.18205600	0.00000000
H	3.27316900	0.45919000	0.00000000
H	2.51749900	1.81281700	-0.89821500
H	4.21755700	-2.96836900	0.00000000

Sum of electronic and zero-point Energies= -871.224636
Sum of electronic and thermal Energies= -871.208110
Sum of electronic and thermal Enthalpies= -871.207166
Sum of electronic and thermal Free Energies= -871.267987

H^+LF(N1) S_0

C	-3.43333700	0.84615600	0.02885800
C	-2.21484200	1.48905400	0.05360100
C	-0.99654800	0.77430900	0.04377900
C	-1.02571200	-0.64960100	0.02432700
C	-2.25856400	-1.30602500	-0.01637800
C	-3.44898000	-0.58398000	-0.01650500
C	1.34026700	-0.61396000	-0.02035000
C	1.28513900	0.81096800	0.00409200
C	2.55965400	1.59517500	-0.00986400
C	3.79024000	-0.56277200	-0.12584200
H	-2.14166100	2.57756300	0.07588300
H	-2.32017100	-2.39167100	-0.07262800
H	4.59711700	1.29961600	-0.08085400
N	0.19538400	-1.31814200	0.04103500
N	2.53882100	-1.22753000	-0.09215400
N	3.70680300	0.80520700	-0.06407000
N	0.15832000	1.46902400	0.04792300
O	2.60375500	2.79331300	0.02438700
O	4.80377600	-1.19894400	-0.20349400
C	-4.75204900	-1.31121000	-0.06998900
H	-5.33454900	-1.00494100	-0.95354100
H	-4.61664000	-2.39913900	-0.10547400
H	-5.37093800	-1.06729400	0.80830200
C	-4.71312500	1.62092100	0.03875700
H	-5.31484400	1.40828400	-0.85879000
H	-5.33327300	1.35371400	0.90875600
H	-4.52370400	2.70071400	0.07410100
H	0.27366200	-3.22569300	-0.88230500
C	0.23978200	-2.77885100	0.12206900
H	1.11149800	-3.08892400	0.71096200
H	-0.64624200	-3.13506100	0.65419300
H	2.63338900	-2.23358200	-0.18440500

Sum of electronic and zero-point Energies= -871.326940
Sum of electronic and thermal Energies= -871.310683
Sum of electronic and thermal Enthalpies= -871.309738
Sum of electronic and thermal Free Energies= -871.370320

H^+LF(N1) S_1

C	-3.45066500	0.82287700	-0.02051500
C	-2.18013800	1.48370800	0.06488600
C	-0.93835500	0.81152500	0.07993300
C	-0.98519900	-0.57649500	0.05761600
C	-2.25383200	-1.25052700	-0.06386900
C	-3.47602400	-0.58542200	-0.08983300
C	1.37323200	-0.54719400	0.03316700
C	1.33128300	0.85340200	0.06470000
C	2.61430300	1.59865800	0.01970300
C	3.81350500	-0.57734800	-0.14239900
H	-2.14256100	2.57401700	0.13399100
H	-2.26333300	-2.33678200	-0.16545400
H	4.64548500	1.27300400	-0.10720600
N	0.20551700	-1.28769300	0.13221300
N	2.54946600	-1.20330200	-0.07508300
N	3.75192400	0.78757100	-0.06866800
N	0.20099800	1.56684200	0.13166900
O	2.69726500	2.79888300	0.05914400
O	4.81326100	-1.23792700	-0.25118000
C	-4.76361600	-1.33820600	-0.20912800
H	-5.32102900	-1.03623300	-1.10989400
H	-4.59382800	-2.42078300	-0.26539500
H	-5.41961600	-1.14452600	0.65442300
C	-4.68979400	1.63039300	-0.04960000
H	-5.26380300	1.42952900	-0.97298800
H	-5.36586700	1.33450600	0.77335300
H	-4.49547500	2.70675900	0.01814900
H	0.26210400	-3.29182900	-0.58967000
C	0.24237900	-2.72492300	0.35523500
H	1.12311800	-2.98105300	0.95867100
H	-0.63075500	-3.02968300	0.94296700
H	2.60354300	-2.21117700	-0.17495100

Sum of electronic and zero-point Energies= -871.222032
Sum of electronic and thermal Energies= -871.204993
Sum of electronic and thermal Enthalpies= -871.204048
Sum of electronic and thermal Free Energies= -871.266664

H^+LF(N1) S_2

C	3.42299800	0.83622000	0.00373800
C	2.21235400	1.50210100	-0.05771500
C	0.97145100	0.82558600	-0.06420900
C	0.99129100	-0.60576700	-0.03179700
C	2.20430500	-1.27621900	0.04880900
C	3.42099800	-0.58345400	0.06946900
C	-1.38088800	-0.57279500	-0.03173200
C	-1.30289800	0.81334000	-0.03699700
C	-2.54663300	1.52330400	0.00088100
C	-3.81185600	-0.56125900	0.08184500
H	2.17043800	2.59165800	-0.09423500
H	2.23817300	-2.36352300	0.11045000
H	-4.59468300	1.34929200	0.07439000
N	-0.24061800	-1.29855500	-0.09123500
N	-2.60091000	-1.20530200	0.03287400
N	-3.70692800	0.84894900	0.04255000
N	-0.16320900	1.54916000	-0.08864100
O	-2.60917200	2.78487400	-0.01158300
O	-4.88084600	-1.09522300	0.15426600
C	4.70610300	-1.34057800	0.16133200
H	5.27921500	-1.04274000	1.05428000
H	4.54060200	-2.42442800	0.20841900
H	5.35305800	-1.13058200	-0.70586400
C	4.71298100	1.59646300	0.01119400
H	5.29254900	1.39002800	0.92477800
H	5.34983700	1.30885000	-0.84018500
H	4.53905900	2.67823400	-0.04424700
H	-0.08926400	-3.24102000	0.75167500
C	-0.24662100	-2.74711700	-0.21940900
H	-1.18344500	-3.09459500	-0.66992400
H	0.55390100	-3.04344300	-0.90795400
H	-2.66914100	-2.21365400	0.11566400

Sum of electronic and zero-point Energies= -871.224478
Sum of electronic and thermal Energies= -871.208060
Sum of electronic and thermal Enthalpies= -871.207116
Sum of electronic and thermal Free Energies= -871.267734

H^+LF(O2-) S_0

C	-2.52707400	2.45957700	0.00000000
C	-2.45018700	1.08569500	0.00000000
C	-1.20737900	0.40959200	0.00000000
C	0.00000000	1.17267300	0.00000000
C	-0.07643100	2.57108200	0.00000000
C	-1.30746200	3.21496000	0.00000000
C	1.21902600	-0.86208100	0.00000000
C	-0.03937600	-1.54025300	0.00000000
C	-0.02714200	-3.02222900	0.00000000
C	2.40722200	-2.78724100	0.00000000
H	-3.34562600	0.46215800	0.00000000
H	0.82800900	3.17710500	0.00000000
H	1.32851100	-4.56606600	0.00000000
N	1.20001600	0.49386400	0.00000000
N	2.40987200	-1.48013100	0.00000000
N	1.28625900	-3.54857000	0.00000000
N	-1.20225400	-0.93448200	0.00000000
O	-0.98090900	-3.74852700	0.00000000
O	3.58672600	-3.36693900	0.00000000
C	-1.36073200	4.70727600	0.00000000
H	-1.90692500	5.07892500	0.88172300
H	-0.35916000	5.15442000	0.00000000
H	-1.90692500	5.07892500	-0.88172300
C	-3.85095000	3.15675200	0.00000000
H	-3.96076300	3.80424100	0.88412400
H	-3.96076300	3.80424100	-0.88412400
H	-4.67867200	2.43694500	0.00000000
H	2.50642500	1.87074500	0.89865600
C	2.45935100	1.24185200	0.00000000
H	3.28300800	0.52432400	0.00000000
H	2.50642500	1.87074500	-0.89865600
H	3.52946900	-4.33368900	0.00000000

Sum of electronic and zero-point Energies= -871.322692
Sum of electronic and thermal Energies= -871.306578
Sum of electronic and thermal Enthalpies= -871.305634
Sum of electronic and thermal Free Energies= -871.365446

H^+LF(O2-) S_1

C	-2.44468300	2.58742400	0.00000000
C	-2.38877300	1.15610500	0.00000000
C	-1.19076400	0.41416200	0.00000000
C	0.00000000	1.14081000	0.00000000
C	-0.04633300	2.57920200	0.00000000
C	-1.23501700	3.30878000	0.00000000
C	1.16611400	-0.92614800	0.00000000
C	-0.09429300	-1.57097200	0.00000000
C	-0.09547400	-3.03674100	0.00000000
C	2.34430400	-2.85931900	0.00000000
H	-3.31729500	0.57961900	0.00000000
H	0.89375100	3.13185500	0.00000000
H	1.23408900	-4.60936100	0.00000000
N	1.20235900	0.46695900	0.00000000
N	2.34940900	-1.54432800	0.00000000
N	1.21826500	-3.59120500	0.00000000
N	-1.27906700	-0.94832400	0.00000000
O	-1.05204200	-3.76936100	0.00000000
O	3.52700600	-3.44051600	0.00000000
C	-1.21909500	4.80482000	0.00000000
H	-1.73585000	5.20937400	0.88487800
H	-0.19430400	5.19694200	0.00000000
H	-1.73585000	5.20937400	-0.88487800
C	-3.76102700	3.26724700	0.00000000
H	-3.85644500	3.93243900	0.87712200
H	-3.85644500	3.93243900	-0.87712200
H	-4.59918000	2.56094300	0.00000000
H	2.56617600	1.79932400	0.90015900
C	2.47560100	1.17389800	0.00000000
H	3.27321600	0.42599200	0.00000000
H	2.56617600	1.79932400	-0.90015900
H	3.46212600	-4.40655800	0.00000000

Sum of electronic and zero-point Energies= -871.220900
Sum of electronic and thermal Energies= -871.204018
Sum of electronic and thermal Enthalpies= -871.203074
Sum of electronic and thermal Free Energies= -871.265043

H^+LF(O2-) S_2

C	-2.48625500	2.56284500	0.00000000
C	-2.46671800	1.17592500	0.00000000
C	-1.25244900	0.47264700	0.00000000
C	0.00000000	1.18313000	0.00000000
C	-0.05010400	2.57151400	0.00000000
C	-1.25943600	3.27541700	0.00000000
C	1.19549700	-0.91828300	0.00000000
C	-0.04690800	-1.60675300	0.00000000
C	-0.07198700	-3.06457100	0.00000000
C	2.36560900	-2.87449700	0.00000000
H	-3.39065900	0.59765200	0.00000000
H	0.87946600	3.14000100	0.00000000
H	1.24926400	-4.62616900	0.00000000
N	1.19075900	0.45034200	0.00000000
N	2.36313300	-1.56835200	0.00000000
N	1.23196400	-3.60848300	0.00000000
N	-1.12413700	-0.84570100	0.00000000
O	-1.05079800	-3.76954300	0.00000000
O	3.54465500	-3.45987400	0.00000000
C	-1.24936700	4.77041700	0.00000000
H	-1.77296300	5.17137800	0.88279800
H	-0.22774600	5.17077500	0.00000000
H	-1.77296300	5.17137800	-0.88279800
C	-3.79241500	3.29367900	0.00000000
H	-3.88098700	3.94477800	0.88391300
H	-3.88098700	3.94477800	-0.88391300
H	-4.64278900	2.60069500	0.00000000
H	2.52363600	1.80468900	0.89847600
C	2.45744000	1.17479800	0.00000000
H	3.27082400	0.44445800	0.00000000
H	2.52363600	1.80468900	-0.89847600
H	3.48192500	-4.42601900	0.00000000

Sum of electronic and zero-point Energies= -871.215308
Sum of electronic and thermal Energies= -871.198607
Sum of electronic and thermal Enthalpies= -871.197663
Sum of electronic and thermal Free Energies= -871.258749

H^+LF(O4+) S_0

C	-2.60737800	2.31395100	0.00000000
C	-2.45524500	0.94817700	0.00000000
C	-1.17657000	0.33949500	0.00000000
C	0.00000000	1.16085100	0.00000000
C	-0.16178900	2.55149800	0.00000000
C	-1.42624300	3.12987800	0.00000000
C	1.36491700	-0.80206200	0.00000000
C	0.11993700	-1.51993400	0.00000000
C	0.21527100	-2.95394500	0.00000000
C	2.66348700	-2.71468200	0.00000000
H	-3.32017500	0.28280500	0.00000000
H	0.70859500	3.20518300	0.00000000
H	1.52735500	-4.50243200	0.00000000
N	1.24090300	0.56718700	0.00000000
N	2.54686900	-1.35680600	0.00000000
N	1.41124200	-3.48823900	0.00000000
N	-1.08537000	-1.00096700	0.00000000
O	-0.84787700	-3.69684000	0.00000000
O	3.67587500	-3.35465400	0.00000000
C	-1.55561200	4.61626500	0.00000000
H	-2.12168200	4.95827300	0.88140600
H	-0.57893700	5.11496400	0.00000000
H	-2.12168200	4.95827300	-0.88140600
C	-3.96557100	2.94180400	0.00000000
H	-4.10955400	3.58239000	0.88416300
H	-4.10955400	3.58239000	-0.88416300
H	-4.75549900	2.18051600	0.00000000
H	2.47566600	2.01254100	0.89951100
C	2.45474200	1.38264000	0.00000000
H	3.31097700	0.70194600	0.00000000
H	2.47566600	2.01254100	-0.89951100
H	-1.62034300	-3.08926900	0.00000000

Sum of electronic and zero-point Energies= -871.319077
Sum of electronic and thermal Energies= -871.303116
Sum of electronic and thermal Enthalpies= -871.302172
Sum of electronic and thermal Free Energies= -871.361722

H^+LF(O4+) S_1

C	-2.52086800	2.42697000	0.00000000
C	-2.40812600	1.01810800	0.00000000
C	-1.18196100	0.35099100	0.00000000
C	0.00000000	1.14497200	0.00000000
C	-0.10957900	2.55385100	0.00000000
C	-1.34095800	3.20936100	0.00000000
C	1.29735200	-0.84187300	0.00000000
C	0.05422300	-1.55904200	0.00000000
C	0.15460300	-2.96339600	0.00000000
C	2.56659000	-2.80359700	0.00000000
H	-3.30918100	0.40159600	0.00000000
H	0.79535100	3.16098900	0.00000000
H	1.44549500	-4.56142500	0.00000000
N	1.23716400	0.52410100	0.00000000
N	2.47905100	-1.42056400	0.00000000
N	1.36127000	-3.54754500	0.00000000
N	-1.16685100	-1.01203400	0.00000000
O	-0.90888700	-3.72204500	0.00000000
O	3.62152300	-3.38665300	0.00000000
C	-1.40693200	4.70335800	0.00000000
H	-1.94707500	5.07867200	0.88393900
H	-0.40579400	5.15248200	0.00000000
H	-1.94707500	5.07867200	-0.88393900
C	-3.86474700	3.06347300	0.00000000
H	-3.98905200	3.71830100	0.87956600
H	-3.98905200	3.71830100	-0.87956600
H	-4.67341700	2.32302600	0.00000000
H	2.51451500	1.93237800	0.89964000
C	2.47394400	1.30310800	0.00000000
H	3.31290200	0.60196600	0.00000000
H	2.51451500	1.93237800	-0.89964000
H	-1.67890800	-3.11317700	0.00000000

Sum of electronic and zero-point Energies= -871.238512
Sum of electronic and thermal Energies= -871.222084
Sum of electronic and thermal Enthalpies= -871.221140
Sum of electronic and thermal Free Energies= -871.281755

H^+LF(O4+) S_2

C	-2.51916700	2.45275500	0.00000000
C	-2.43123400	1.07152400	0.00000000
C	-1.19058700	0.40031800	0.00000000
C	0.00000000	1.18549500	0.00000000
C	-0.08408800	2.56986700	0.00000000
C	-1.32333100	3.22068300	0.00000000
C	1.27918800	-0.81456800	0.00000000
C	0.04393900	-1.56314000	0.00000000
C	0.14429100	-2.95709000	0.00000000
C	2.58506300	-2.89952800	0.00000000
H	-3.33101400	0.45476100	0.00000000
H	0.81760400	3.18119700	0.00000000
H	1.40116400	-4.58678100	0.00000000
N	1.24528300	0.51313500	0.00000000
N	2.38002000	-1.53146400	0.00000000
N	1.34757900	-3.56983300	0.00000000
N	-1.14090200	-0.94476700	0.00000000
O	-0.91368700	-3.73008800	0.00000000
O	3.64103600	-3.45726100	0.00000000
C	-1.37988200	4.71402800	0.00000000
H	-1.92249100	5.09051500	0.88221900
H	-0.37786500	5.16127600	0.00000000
H	-1.92249100	5.09051500	-0.88221900
C	-3.85528000	3.12840400	0.00000000
H	-3.97384400	3.77477100	0.88382000
H	-3.97384400	3.77477100	-0.88382000
H	-4.67405700	2.39818200	0.00000000
H	2.54907800	1.89920200	0.89875500
C	2.49479900	1.27046000	0.00000000
H	3.33437400	0.56527600	0.00000000
H	2.54907800	1.89920200	-0.89875500
H	-1.70060700	-3.14884300	0.00000000

Sum of electronic and zero-point Energies= -871.217562
Sum of electronic and thermal Energies= -871.201359
Sum of electronic and thermal Enthalpies= -871.200415
Sum of electronic and thermal Free Energies= -871.260296

H^+LF(N5) S_0

C	-2.60490600	2.32358600	0.00000000
C	-2.45868900	0.95216400	0.00000000
C	-1.18185800	0.36945300	0.00000000
C	0.00000000	1.15995500	0.00000000
C	-0.16280300	2.55180600	0.00000000
C	-1.42454100	3.13569400	0.00000000
C	1.37621600	-0.82347000	0.00000000
C	0.15080900	-1.56821600	0.00000000
C	0.16529200	-3.05077300	0.00000000
C	2.63559800	-2.77263200	0.00000000
H	-3.33596500	0.30117000	0.00000000
H	0.71170700	3.19969900	0.00000000
H	1.55737300	-4.54681300	0.00000000
N	1.23843800	0.55482000	0.00000000
N	2.54062300	-1.38731800	0.00000000
N	1.42839300	-3.53615800	0.00000000
N	-1.01657700	-0.98527300	0.00000000
O	-0.88154800	-3.66824600	0.00000000
O	3.68221500	-3.36020100	0.00000000
C	-1.54971200	4.62322500	0.00000000
H	-2.11258700	4.96824500	0.88208900
H	-0.57071400	5.11729100	0.00000000
H	-2.11258700	4.96824500	-0.88208900
C	-3.96241100	2.95021600	0.00000000
H	-4.10328700	3.59185800	0.88389500
H	-4.10328700	3.59185800	-0.88389500
H	-4.75547100	2.19220500	0.00000000
H	2.48134300	1.99414500	0.90011500
C	2.45520700	1.36459200	0.00000000
H	3.30719400	0.67773400	0.00000000
H	2.48134300	1.99414500	-0.90011500
H	-1.81574100	-1.63831400	0.00000000

Sum of electronic and zero-point Energies= -871.312878
Sum of electronic and thermal Energies= -871.296823
Sum of electronic and thermal Enthalpies= -871.295879
Sum of electronic and thermal Free Energies= -871.355815

H^+LF(N5) S_1

C	-2.51077800	2.44762900	0.00000000
C	-2.42293000	1.04124100	0.00000000
C	-1.20171500	0.38290300	0.00000000
C	0.00000000	1.13727200	0.00000000
C	-0.09582000	2.54402100	0.00000000
C	-1.31866900	3.21142300	0.00000000
C	1.28480800	-0.87075900	0.00000000
C	0.06950000	-1.61882200	0.00000000
C	0.09011700	-3.06553400	0.00000000
C	2.55043000	-2.85313900	0.00000000
H	-3.34097800	0.44921000	0.00000000
H	0.81598900	3.13977300	0.00000000
H	1.46605900	-4.59938400	0.00000000
N	1.22977100	0.49418300	0.00000000
N	2.46785400	-1.44580300	0.00000000
N	1.36852100	-3.58686300	0.00000000
N	-1.12403400	-0.98840100	0.00000000
O	-0.93291800	-3.72704300	0.00000000
O	3.63233200	-3.38673900	0.00000000
C	-1.36629400	4.70655900	0.00000000
H	-1.90173500	5.08745400	0.88413500
H	-0.35978400	5.14323700	0.00000000
H	-1.90173500	5.08745400	-0.88413500
C	-3.84496100	3.10697000	0.00000000
H	-3.95773700	3.76188000	0.88038100
H	-3.95773700	3.76188000	-0.88038100
H	-4.66676200	2.38094600	0.00000000
H	2.51203100	1.89624100	0.90011100
C	2.47170000	1.26756000	0.00000000
H	3.30621600	0.56100000	0.00000000
H	2.51203100	1.89624100	-0.90011100
H	-1.94829900	-1.59141900	0.00000000

Sum of electronic and zero-point Energies= -871.241701
Sum of electronic and thermal Energies= -871.225913
Sum of electronic and thermal Enthalpies= -871.224968
Sum of electronic and thermal Free Energies= -871.284244

H^+LF(N5) S_2

C	-2.52838300	2.42852000	0.00000000
C	-2.44759800	1.04742900	0.00000000
C	-1.20811700	0.39201000	0.00000000
C	0.00000000	1.14312200	0.00000000
C	-0.09226400	2.53808600	0.00000000
C	-1.32137800	3.19025500	0.00000000
C	1.29215600	-0.87914700	0.00000000
C	0.08155800	-1.60074800	0.00000000
C	0.10008100	-3.04164200	0.00000000
C	2.51126600	-2.78486500	0.00000000
H	-3.35823800	0.44450300	0.00000000
H	0.81339800	3.14162800	0.00000000
H	1.48257200	-4.58748400	0.00000000
N	1.22785100	0.48276900	0.00000000
N	2.49182900	-1.45798200	0.00000000
N	1.39694200	-3.57354800	0.00000000
N	-1.11822700	-0.96275800	0.00000000
O	-0.88347400	-3.75007100	0.00000000
O	3.61330800	-3.41248300	0.00000000
C	-1.37473900	4.68352800	0.00000000
H	-1.91624000	5.05997300	0.88264100
H	-0.37131800	5.12684600	0.00000000
H	-1.91624000	5.05997300	-0.88264100
C	-3.85815100	3.11130000	0.00000000
H	-3.96960700	3.75977500	0.88331600
H	-3.96960700	3.75977500	-0.88331600
H	-4.68388200	2.38909300	0.00000000
H	2.50068000	1.89201100	0.89879200
C	2.46369600	1.26099400	0.00000000
H	3.30246900	0.56068200	0.00000000
H	2.50068000	1.89201100	-0.89879200
H	-1.95087200	-1.55078000	0.00000000

Sum of electronic and zero-point Energies= -871.245759
Sum of electronic and thermal Energies= -871.229554
Sum of electronic and thermal Enthalpies= -871.228610
Sum of electronic and thermal Free Energies= -871.288633

H^+LF(OH++) S_0

C	-2.58116400	2.34865400	0.00000000
C	-2.45213900	0.98027500	0.00000000
C	-1.18422500	0.35005800	0.00000000
C	0.00000000	1.15843800	0.00000000
C	-0.13532300	2.55324300	0.00000000
C	-1.38874800	3.15016400	0.00000000
C	1.30951000	-0.81976800	0.00000000
C	0.07767500	-1.53927500	0.00000000
C	0.20131600	-2.98687000	0.00000000
C	2.43717300	-2.76938400	0.00000000
H	-3.32706700	0.32831200	0.00000000
H	0.74548600	3.19305500	0.00000000
N	1.22889700	0.53859100	0.00000000
N	2.48778900	-1.43171500	0.00000000
N	1.36141200	-3.57998400	0.00000000
N	-1.11730900	-0.99187000	0.00000000
O	-0.88643200	-3.71072100	0.00000000
O	3.57893700	-3.40979600	0.00000000
C	-1.49847000	4.63858400	0.00000000
H	-2.05905200	4.98867100	0.88159800
H	-0.51489600	5.12373900	0.00000000
H	-2.05905200	4.98867100	-0.88159800
C	-3.92951700	2.99636300	0.00000000
H	-4.06265500	3.63942600	0.88408500
H	-4.06265500	3.63942600	-0.88408500
H	-4.73087700	2.24731300	0.00000000
H	2.48682200	1.96215700	0.89910100
C	2.45773500	1.33256000	0.00000000
H	3.30393500	0.64127500	0.00000000
H	2.48682200	1.96215700	-0.89910100
H	4.29473600	-2.75240300	0.00000000
H	-1.65006400	-3.10107100	0.00000000

Sum of electronic and zero-point Energies= -871.322326
Sum of electronic and thermal Energies= -871.306536
Sum of electronic and thermal Enthalpies= -871.305592
Sum of electronic and thermal Free Energies= -871.364672

H^+LF(OH++) S_1

C	-2.50601100	2.47214600	0.00000000
C	-2.39489400	1.04728100	0.00000000
C	-1.17081200	0.35463400	0.00000000
C	0.00000000	1.12646300	0.00000000
C	-0.10652500	2.55778000	0.00000000
C	-1.32470600	3.23888400	0.00000000
C	1.26434900	-0.87710500	0.00000000
C	0.02607200	-1.57286300	0.00000000
C	0.13965900	-2.99995100	0.00000000
C	2.37213900	-2.85197300	0.00000000
H	-3.30341900	0.44028400	0.00000000
H	0.80970400	3.14899100	0.00000000
N	1.23211100	0.51103300	0.00000000
N	2.42844400	-1.49419200	0.00000000
N	1.30098900	-3.63061900	0.00000000
N	-1.19058200	-1.01178300	0.00000000
O	-0.95734300	-3.71852900	0.00000000
O	3.52870300	-3.47595500	0.00000000
C	-1.36698100	4.73400000	0.00000000
H	-1.90010400	5.11724100	0.88467800
H	-0.35876200	5.16676800	0.00000000
H	-1.90010400	5.11724100	-0.88467800
C	-3.84738800	3.10344700	0.00000000
H	-3.96823800	3.76345900	0.87758100
H	-3.96823800	3.76345900	-0.87758100
H	-4.65879800	2.36643500	0.00000000
H	2.54411400	1.89552800	0.90049300
C	2.47645600	1.26825900	0.00000000
H	3.29971200	0.54848100	0.00000000
H	2.54411400	1.89552800	-0.90049300
H	4.23039100	-2.80499800	0.00000000
H	-1.70614100	-3.08963300	0.00000000

Sum of electronic and zero-point Energies= -871.227728
Sum of electronic and thermal Energies= -871.211247
Sum of electronic and thermal Enthalpies= -871.210303
Sum of electronic and thermal Free Energies= -871.271218

H^+LF(OH++) S_2

C	-2.51232300	2.45678400	0.00000000
C	-2.43809100	1.07438700	0.00000000
C	-1.20946300	0.38727500	0.00000000
C	0.00000000	1.15543500	0.00000000
C	-0.07566600	2.54454900	0.00000000
C	-1.30556600	3.20868300	0.00000000
C	1.24549400	-0.86715000	0.00000000
C	0.00926700	-1.53993700	0.00000000
C	0.10403800	-2.96507800	0.00000000
C	2.44543600	-2.87903400	0.00000000
H	-3.34415500	0.46666900	0.00000000
H	0.83208600	3.14651100	0.00000000
N	1.23716800	0.48711200	0.00000000
N	2.39485500	-1.56307800	0.00000000
N	1.29471700	-3.53506000	0.00000000
N	-1.19011100	-0.96748000	0.00000000
O	-0.96971200	-3.70158400	0.00000000
O	3.55619200	-3.56949600	0.00000000
C	-1.34460600	4.70280000	0.00000000
H	-1.88291000	5.08542500	0.88218300
H	-0.33726000	5.13794800	0.00000000
H	-1.88291000	5.08542500	-0.88218300
C	-3.83977500	3.14845700	0.00000000
H	-3.95137400	3.79648900	0.88367200
H	-3.95137400	3.79648900	-0.88367200
H	-4.66689000	2.42766600	0.00000000
H	2.53692900	1.87581400	0.89719300
C	2.48035700	1.24326100	0.00000000
H	3.32051400	0.54265700	0.00000000
H	2.53692900	1.87581400	-0.89719300
H	4.31509700	-2.96411300	0.00000000
H	-1.72753100	-3.07720300	0.00000000

Sum of electronic and zero-point Energies= -871.227425
Sum of electronic and thermal Energies= -871.211061
Sum of electronic and thermal Enthalpies= -871.210116
Sum of electronic and thermal Free Energies= -871.270326

H^+LF(OH+-) S_0

C	-2.56819800	2.38408700	0.00000000
C	-2.45271000	1.01502100	0.00000000
C	-1.18986200	0.37078200	0.00000000
C	0.00000000	1.16901000	0.00000000
C	-0.11914000	2.56504600	0.00000000
C	-1.36746600	3.17330700	0.00000000
C	1.27796600	-0.82853300	0.00000000
C	0.03605600	-1.53933500	0.00000000
C	0.17565400	-2.98346800	0.00000000
C	2.42192200	-2.76906400	0.00000000
H	-3.33036700	0.36671700	0.00000000
H	0.76749800	3.19680000	0.00000000
N	1.21778000	0.53085900	0.00000000
N	2.46191100	-1.43815300	0.00000000
N	1.34078300	-3.57351000	0.00000000
N	-1.15068700	-0.96870100	0.00000000
O	-0.92308900	-3.69067100	0.00000000
O	3.56252500	-3.41437300	0.00000000
C	-1.46269000	4.66282900	0.00000000
H	-2.02011800	5.01816900	0.88150200
H	-0.47452200	5.13864800	0.00000000
H	-2.02011800	5.01816900	-0.88150200
C	-3.91014300	3.04570500	0.00000000
H	-4.03757900	3.68976000	0.88422000
H	-4.03757900	3.68976000	-0.88422000
H	-4.71809100	2.30377000	0.00000000
H	2.48989200	1.94101400	0.89879300
C	2.45531900	1.31129700	0.00000000
H	3.29524900	0.61308500	0.00000000
H	2.48989200	1.94101400	-0.89879300
H	4.27958000	-2.75848100	0.00000000
H	-0.66797900	-4.63164600	0.00000000

Sum of electronic and zero-point Energies= -871.324135
Sum of electronic and thermal Energies= -871.308301
Sum of electronic and thermal Enthalpies= -871.307357
Sum of electronic and thermal Free Energies= -871.366574

H^+LF(OH+-) S_1

C	-2.48706900	2.51379400	0.00000000
C	-2.39224900	1.08689000	0.00000000
C	-1.17504000	0.37943800	0.00000000
C	0.00000000	1.13905000	0.00000000
C	-0.08678000	2.57317700	0.00000000
C	-1.29648300	3.26797800	0.00000000
C	1.22974900	-0.88912100	0.00000000
C	-0.02306300	-1.57412700	0.00000000
C	0.10701900	-2.99938100	0.00000000
C	2.35246700	-2.85279100	0.00000000
H	-3.30461500	0.48530800	0.00000000
H	0.83653100	3.15334100	0.00000000
N	1.21855200	0.50120500	0.00000000
N	2.39776100	-1.50262300	0.00000000
N	1.27565900	-3.62407700	0.00000000
N	-1.22512800	-0.98345800	0.00000000
O	-0.99427000	-3.71512100	0.00000000
O	3.50741200	-3.48267600	0.00000000
C	-1.32259800	4.76356700	0.00000000
H	-1.85122000	5.15297400	0.88470400
H	-0.30955200	5.18501900	0.00000000
H	-1.85122000	5.15297400	-0.88470400
C	-3.82107300	3.15952700	0.00000000
H	-3.93450600	3.82125500	0.87741200
H	-3.93450600	3.82125500	-0.87741200
H	-4.64012600	2.43110300	0.00000000
H	2.54811000	1.86826100	0.90029100
C	2.47309400	1.24152300	0.00000000
H	3.28770100	0.51263300	0.00000000
H	2.54811000	1.86826100	-0.90029100
H	4.21043200	-2.81326700	0.00000000
H	-0.72603600	-4.65121500	0.00000000

Sum of electronic and zero-point Energies= -871.228114
Sum of electronic and thermal Energies= -871.211546
Sum of electronic and thermal Enthalpies= -871.210602
Sum of electronic and thermal Free Energies= -871.271793

H^+LF(OH+-) S_2

C	-2.51914700	2.49006200	0.00000000
C	-2.45782800	1.10628400	0.00000000
C	-1.22555300	0.43097300	0.00000000
C	0.00000000	1.18059500	0.00000000
C	-0.08134200	2.56915400	0.00000000
C	-1.30973100	3.23665500	0.00000000
C	1.25071800	-0.87401100	0.00000000
C	0.00886000	-1.58752400	0.00000000
C	0.11915900	-3.01099800	0.00000000
C	2.38891300	-2.88022000	0.00000000
H	-3.36564300	0.50245200	0.00000000
H	0.82982200	3.16625900	0.00000000
N	1.21510600	0.48796400	0.00000000
N	2.38836100	-1.54748700	0.00000000
N	1.28595500	-3.61838000	0.00000000
N	-1.10578300	-0.89682400	0.00000000
O	-1.00506000	-3.69789000	0.00000000
O	3.53033400	-3.53088500	0.00000000
C	-1.34287500	4.73104700	0.00000000
H	-1.87886400	5.11602800	0.88250700
H	-0.33360300	5.16156000	0.00000000
H	-1.87886400	5.11602800	-0.88250700
C	-3.84380000	3.18670200	0.00000000
H	-3.95085400	3.83515600	0.88383500
H	-3.95085400	3.83515600	-0.88383500
H	-4.67485500	2.47059700	0.00000000
H	2.51983900	1.87148200	0.89821000
C	2.46358300	1.24047500	0.00000000
H	3.29374400	0.52856800	0.00000000
H	2.51983900	1.87148200	-0.89821000
H	4.25990900	-2.89113500	0.00000000
H	-0.78300400	-4.64552100	0.00000000

Sum of electronic and zero-point Energies= -871.225108
Sum of electronic and thermal Energies= -871.208552
Sum of electronic and thermal Enthalpies= -871.207607
Sum of electronic and thermal Free Energies= -871.268219

H^+LF(O4-) S_0

C	-2.59678500	2.34258500	0.00000000
C	-2.45480600	0.97626500	0.00000000
C	-1.17911900	0.35658600	0.00000000
C	0.00000000	1.17093800	0.00000000
C	-0.14816300	2.56280600	0.00000000
C	-1.40920400	3.14940900	0.00000000
C	1.33729000	-0.81034100	0.00000000
C	0.08342400	-1.52675400	0.00000000
C	0.19223600	-2.96198100	0.00000000
C	2.65805700	-2.70171600	0.00000000
H	-3.32057600	0.31205400	0.00000000
H	0.72655900	3.21066700	0.00000000
H	1.56059500	-4.48648000	0.00000000
N	1.23022900	0.55970900	0.00000000
N	2.52802500	-1.35376600	0.00000000
N	1.40230600	-3.47858100	0.00000000
N	-1.11309300	-0.98075900	0.00000000
O	-0.90342300	-3.66535400	0.00000000
O	3.66653100	-3.34966000	0.00000000
C	-1.52787300	4.63680400	0.00000000
H	-2.09173600	4.98269700	0.88130900
H	-0.54771000	5.12870100	0.00000000
H	-2.09173600	4.98269700	-0.88130900
C	-3.95033400	2.98116900	0.00000000
H	-4.09019500	3.62251100	0.88429800
H	-4.09019500	3.62251100	-0.88429800
H	-4.74509600	2.22493600	0.00000000
H	2.47529100	1.99521400	0.89922100
C	2.45126000	1.36510600	0.00000000
H	3.30330200	0.68002200	0.00000000
H	2.47529100	1.99521400	-0.89922100
H	-0.73681400	-4.62210200	0.00000000

Sum of electronic and zero-point Energies= -871.307077
Sum of electronic and thermal Energies= -871.290966
Sum of electronic and thermal Enthalpies= -871.290022
Sum of electronic and thermal Free Energies= -871.349883

H^+LF(O4-) S_1

C	-2.50727900	2.46038900	0.00000000
C	-2.40241900	1.04684200	0.00000000
C	-1.18069600	0.37141200	0.00000000
C	0.00000000	1.15601900	0.00000000
C	-0.09693900	2.56918800	0.00000000
C	-1.32311900	3.23454400	0.00000000
C	1.27130500	-0.85376700	0.00000000
C	0.01314500	-1.56717400	0.00000000
C	0.12738300	-2.97631300	0.00000000
C	2.55922500	-2.79134700	0.00000000
H	-3.30499100	0.43221400	0.00000000
H	0.81324300	3.16860300	0.00000000
H	1.48223400	-4.54837500	0.00000000
N	1.22371700	0.51849500	0.00000000
N	2.45627400	-1.41810500	0.00000000
N	1.35320600	-3.53987600	0.00000000
N	-1.19021400	-0.99062900	0.00000000
O	-0.96794100	-3.70068200	0.00000000
O	3.61016100	-3.38219500	0.00000000
C	-1.37832100	4.72929400	0.00000000
H	-1.91520300	5.10884100	0.88409400
H	-0.37373500	5.17076200	0.00000000
H	-1.91520300	5.10884100	-0.88409400
C	-3.84745500	3.10254600	0.00000000
H	-3.96827700	3.75902800	0.87915700
H	-3.96827700	3.75902800	-0.87915700
H	-4.65967300	2.36609800	0.00000000
H	2.51578400	1.91348400	0.89961800
C	2.46869000	1.28459500	0.00000000
H	3.30089600	0.57603800	0.00000000
H	2.51578400	1.91348400	-0.89961800
H	-0.78234500	-4.65158500	0.00000000

Sum of electronic and zero-point Energies= -871.224855
Sum of electronic and thermal Energies= -871.208089
Sum of electronic and thermal Enthalpies= -871.207144
Sum of electronic and thermal Free Energies= -871.268480

H^+LF(O4-) S_2

C	-2.53083800	2.46227500	0.00000000
C	-2.44808300	1.08165100	0.00000000
C	-1.20276900	0.42045300	0.00000000
C	0.00000000	1.19331800	0.00000000
C	-0.09330200	2.57941000	0.00000000
C	-1.33221800	3.22817700	0.00000000
C	1.28556400	-0.83345900	0.00000000
C	0.03160100	-1.59176000	0.00000000
C	0.13557200	-2.98733300	0.00000000
C	2.58602900	-2.85203300	0.00000000
H	-3.34640000	0.46357800	0.00000000
H	0.80864900	3.19012800	0.00000000
H	1.47304100	-4.57338000	0.00000000
N	1.22525800	0.51116500	0.00000000
N	2.40652500	-1.49178000	0.00000000
N	1.35838000	-3.56264300	0.00000000
N	-1.09832900	-0.90834600	0.00000000
O	-0.97642600	-3.69516600	0.00000000
O	3.63603600	-3.42906400	0.00000000
C	-1.38833600	4.72157500	0.00000000
H	-1.93064100	5.09815100	0.88235100
H	-0.38599200	5.16795800	0.00000000
H	-1.93064100	5.09815100	-0.88235100
C	-3.86589900	3.13997300	0.00000000
H	-3.98298100	3.78638900	0.88397000
H	-3.98298100	3.78638900	-0.88397000
H	-4.68600900	2.41127200	0.00000000
H	2.52342900	1.90176800	0.89901800
C	2.47292700	1.27264800	0.00000000
H	3.30767400	0.56334200	0.00000000
H	2.52342900	1.90176800	-0.89901800
H	-0.81178100	-4.64981700	0.00000000

Sum of electronic and zero-point Energies= -871.211420
Sum of electronic and thermal Energies= -871.194830
Sum of electronic and thermal Enthalpies= -871.193885
Sum of electronic and thermal Free Energies= -871.254532